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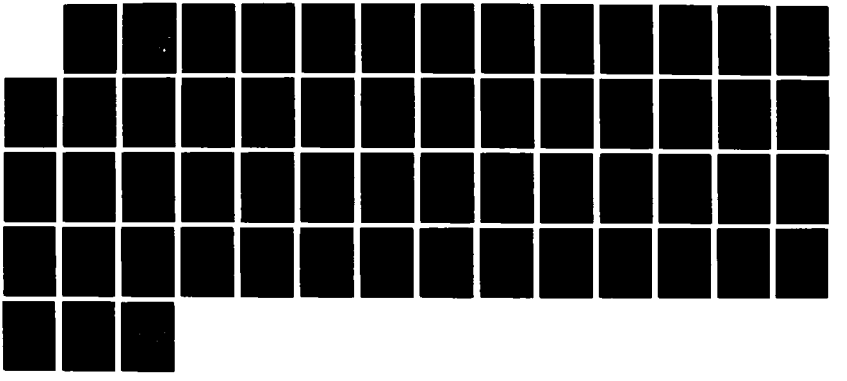

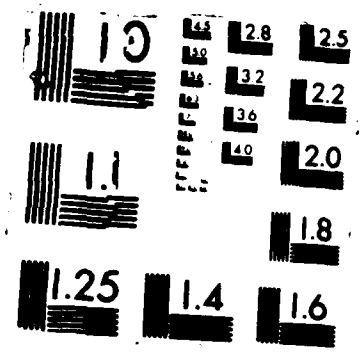
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Analysis of the Spectra of Triply Ionized Iron in Rare-Earth Aluminum Garnets

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Experimental data on the spectra of Fe^{3+} in seven rare-earth aluminum garnets are analyzed. The first analysis consists of the conventional cubic approximations to obtain the Slater parameters $F^{(2)}$, $F^{(4)}$ and the crystal field parameters B_{40}. The concept of rotational invariance of the crystal fields, along with the point charge lattice sums, was used to predict the crystal field parameters for the Al_2 site with C_{3i} symmetry. The best fit Slater parameters, along with the spin-orbit parameter, were used to predict the optical spectra of Fe^{3+} in $R_3Al_5O_{12}$ for R = Gd, Tb, Dy Ho, Er, Tm, Yb, and Lu.

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1. INTRODUCTION

Recent successes in transferring energy from excited chromium ions to neodymium ions in gadolinium scandium gallium garnets have increased interest in the spectra of transition-metal ions in potential laser host materials [1-4].* In particular, the garnet materials, which can be doped with both rare-earth and transition-metal ions, are possible candidates for such a laser.

In the work reported here, we analyze the spectra of Fe^{3+} in the rare-earth aluminum garnets, $R_3Al_5O_{12}$ (RAG), for R = Gd, Tb, Dy, Ho, Er, Tm, and Yb [5]. The Fe^{3+} ion is assumed to occupy the 6(a) site with C_{3i} symmetry [6]. The reported analysis of the experimental data [5] assumes cubic symmetry and gives the usual parameters (B, C, and Dq) for the free ion and the crystal field. Using the known crystallographic data [7] on RAG, we then compute the crystal field components, A_{nm}. The concept of rotational invariance is used [8] to obtain an estimate of the radial integrals needed to convert the crystal field components to the crystal field parameters, B_{nm}. The resulting crystal field parameters are used to calculate the energy levels of Fe^{3+} in the entire RAG series, including lutetium. This latter calculation is performed with the spin-orbit constant, ζ, equal to 370 cm^{-1}, which we assume is approximately 80 percent of the free ion value [9].

2. THEORY

The interactions of the free ion considered here for the d^N electronic configuration are the coulomb interaction, the spin-orbit interaction, and the configuration interaction. Although these interactions are tabulated in numerous places, we include a brief discussion here for completeness.

The coulomb interaction for the configuration d^N is given by

$$H_1 = \sum_{\substack{k=0 \\ k\ \text{even}}}^{4} F^{(k)} \sum_{\substack{i>j \\ m}}^{N} C^*_{km}(i) C_{km}(j) , \tag{1}$$

where the $F^{(k)}$ are the Slater parameters. The $C_{km}(i)$ in equation (1) are related to the ordinary spherical harmonics by

$$C_{km}(i) = [4\pi/2k + 1]^{1/2} Y_{km}(\theta_i, \phi_i) . \tag{2}$$

The Slater integrals are related to the Racah parameters B and C [10] by

$$\begin{aligned} F^{(2)} &= 7(7B + C) \\ F^{(4)} &= 63C/5 . \end{aligned} \tag{3}$$

*References appear at the end of the report (p 50).

The Slater parameter $F^{(0)}$ and the Racah parameter A are ignored in our analysis. The spin-orbit interaction for the d^N configuration is taken as

$$H_2 = \zeta \sum_{i=1}^{N} \vec{s}_i \cdot \vec{\ell}_i \ , \tag{4}$$

where $\vec{s}_i$ and $\vec{\ell}_i$ are the spin and orbital angular momentum operators. Values of $F^{(k)}$ and ζ calculated with the use of nonrelativistic Hartree-Fock wave functions for a large number of ions with the nd^N configurations are given by Fraga et al [11]. For Fe^{3+} their values (in cm^{-1}) are

$$F^{(2)}_{HF} = 99,367 \ , \ F^{(4)}_{HF} = 62,291 \ , \text{ and } \zeta_{HF} = 499.53 \ .$$

For the free ion, Uylings et al [9] give (in cm^{-1}) $F^{(2)} = 83,302$, $F^{(4)} = 53,070$, and $\zeta = 463$ (other parameters used by Uylings et al are (in cm^{-1}) $\alpha = 35.40$, $\beta = -486.7$, and $T = -6.2$).

For the interconfiguration interaction we take the form suggested by the work of Rajnak and Wybourne [12] as

$$H_3 = \alpha L(L + 1) + \gamma G(R_5) \ , \tag{5}$$

which is a form previously suggested by Trees [13]. However, in the form suggested by Trees, the second term in equation (5) involves the seniority operator Q with the parameter β instead of the Casimir operator $G(R_5)$. Unfortunately, the inclusion of either form (βQ or $\gamma G(R_5)$) in a fitting of the experimental data generally gives erratic values for β or γ. That is, small changes in the experimental data give large changes in the values of γ or β so that this interaction is frequently ignored. On the other hand, the inclusion of the term involving α in equation (5) frequently improves the fit to the experimental data, and the value found by fitting generally is positive and less than 100 cm^{-1}. The crystal field interaction for the d^N electronic configuration in the C_{3i} site in $R_3Al_5O_{12}$ is taken as

$$H_4 = B_{20} \sum_{i=1}^{w} C_{20}(i) + B_{40} \sum_{i=1}^{n} C_{40}(i) + B_{43} \sum_{i=1}^{n} [C_{43}(i) - C_{4-3}(i)] \ , \tag{6}$$

where the B_{nm} are the crystal field parameters and the $C_{nm}(i)$ are given in equation (2). In equation (6) the crystal field parameter B_{43} has been chosen real and can be further chosen positive or negative with no loss in generality. In the cubic approximation we have

$$B_{20} = 0 \ ,$$

$$B_{40} = -14Dq \ , \tag{7}$$

and

$$B_{43} = \sqrt{10/7}\ B_{40} \ ,$$

where Dq is the more familiar crystal field parameter used in the analysis of the spectra of ions with the d^N electronic configuration. The relation of the crystal field parameters of equation (6) to the parameters given by Macfarlane [14] are

$$B_{20} = (7v - 2w)/3 ,$$

$$B_{40} = -7Dq/5 + 2w/3 , \tag{8}$$

and

$$B_{43} = -\sqrt{7/10}\ (2Dq + w/3) ,$$

where $w = 2v + 3\sqrt{2}\ v'$, and it should be noted that this relation gives $B_{43} < 0$ since the value of Dq is usually chosen positive. In obtaining the result given in equation (8), we have used the relations

$$\sum_{i=1}^{N} C_{2m}(i) = -\sqrt{2/7}\ U_m^{(2)}$$

$$\sum_{i=1}^{N} C_{4m}(i) = \sqrt{2/7}\ U_m^{(4)} \quad , \tag{9}$$

where the $U_m^{(n)}$ are the unit tensors introduced by Racah [10] and are identical to those used by Nielson and Koster [15]. The relation of other conventions used for the crystal field parameters for the electronic configuration d^N are given by Konig and Kremer [16]. The complete Hamiltonian we consider is

$$H = \sum_{i=1}^{4} H_i \ . \tag{10}$$

3. WAVE FUNCTIONS AND FITTING THE EXPERIMENTAL DATA

Because of the large variation in the relative strength of the various interactions occurring in H_1 through H_5, we decided to use total angular momentum wave functions, J, as a basis for calculating the energy levels of Fe^{3+} in RAG. That is, the wave functions are $|JM\alpha LS\rangle$, with $\underline{J} = \underline{L} + \underline{S}$, and α represents the additional quantum numbers needed to uniquely specify the states. In C_3 or C_{3i} symmetry, the states given by $M = 1/2 + 3q$ ($q = 0, \pm1\ldots$) and $M = -1/2 + 3q$ ($q = 0, \pm1\ldots$) are degenerate and correspond to the Γ_4 and Γ_5 irreducible representations of the C_{3i} group, respectively. The states with $M = 3/2 + 3q$ ($q = 0, \pm1$), which correspond to the Γ_6 irreducible representation, are chosen as

$$\psi_6^+ = (|JM\alpha LS\rangle + (-1)^{J-M}\ |J - M\alpha LS\rangle)/\sqrt{2}$$

$$\psi_6^- = (|JM\alpha LS\rangle - (-1)^{J-M}\ |J - M\alpha LS\rangle)/\sqrt{2} \ , \tag{11}$$

and the energy levels obtained by using ψ_6^+ or ψ_6^- are degenerate. The matrix for H in the states $|JM\alpha LS\rangle$ for M = 1/2 + 3q is 84 × 84, and for the ψ_6^+ is 42 × 42.

3.1 Cubic Approximation

The experimental data on Fe^{3+} in RAG with R = Gd, Tb, Dy, Ho, Er, Tm, and Yb have been reported by Arsenev et al [5]. In their analysis, they assumed cubic symmetry and reported the crystal field parameter Dq and the Racah parameters B and C, as well as the experimental and theoretical energy levels. These parameters were converted to $F^{(k)}$ and B_{nm} with the use of equations (3) and (7) and are given in table 1 in the row labeled 1. As can be seen, the rms deviation of the theoretical from the experimental levels is quite large, and it was assumed that there was a misprint or that one or more levels were mislabeled. To try to resolve this possible discrepancy, we used the reported theoretical energy levels as data and varied the parameters to obtain a best fit, with the results given in table 1, row 2. Despite a number of different reasonable selections of level changes and other possible changes, we were unable to obtain what we considered a satisfactory result. It was then decided to best fit the experimental data starting with the parameters given in row 1 of table 1. The results are given in row 3 of table 1, and, as is shown, the resulting fits to Gd through Yb are very good. With the use of the parameters given in row 3 of table 1, tables 2 through 8 give the energy levels of Fe^{3+} for all the compounds. In these tables the familiar Mulligen notation is used for the irreducible representation. It was decided to proceed with the analysis and prediction using the results of row 3, table 1.

TABLE 1. SLATER PARAMETERS $F^{(k)}$ AND CRYSTAL FIELD PARAMETERS (CUBIC) B_{40}, B_{43} FOR Fe^{3+} ION IN $R_3Al_5O_{12}$

R	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	B_{40} (cm^{-1})	B_{43} (cm^{-1})	rms (cm^{-1})	Row No.
Gd	53305	41706	-19110	22840.82	725.0	1
Gd	51732	37897	-19198	22945.94	464.0	2
Gd	52406	42491	-21441	25627.23	78.7	3
Tb	53501	41618	-19320	23091.82	686.0	1
Tb	52538	37825	-19312	23082.19	409.0	2
Tb	52553	42403	-21521	25722.10	84.1	3
Dy	53872	41403	-20160	24095.81	600.0	1
Dy	53355	38773	-20134	24064.53	278.0	2
Dy	52934	42164	-21668	25898.31	86.7	3
Ho	53963	41391	-20370	24346.81	436.0	1
Ho	53464	38954	-20332	24301.39	272.0	2
Ho	53126	42039	-21757	26004.29	81.1	3
Er	54362	41139	-21000	25099.80	463.0	1
Er	53535	42184	-20903	24983.66	318.0	2
Er	53522	41738	-21882	26153.99	89.9	3
Tm	54488	41101	-21574	25785.86	476.0	1
Tm	53477	42968	-21447	25633.62	314.0	2
Tm	53672	41654	-21963	26250.80	91.5	3
Yb	54663	41063	-21840	26103.79	146.0	1
Yb	54929	40773	-21829	26090.30	116.0	2
Yb	53876	41567	-22065	26372.72	97.3	3

1--Parameters reported by Arsenev et al [5].

2--Best-fit parameters obtained by fitting the theoretical levels of Arsenev et al [5].

3--Best-fit parameters obtained by fitting the experimental data of Arsenev et al [5].

TABLE 2. ENERGY LEVELS OF Fe^{3+} IN $Gd_3Al_5O_{12}$

[Theoretical levels were calculated with $F^{(2)} = 52406$, $F^{(4)} = 42491$, and $B_{40} = -21441$ (Dq = 1531.5, B = 587.75, and C = 3372.3). All quantities are in cm^{-1}.]

No.	IR*	†E_{obs}	E_{th}	Free ion state composition
1	$^6A_1$	0	-3	1.00 6S
2	$^2T_2$	0	9511	0.31 2I + 0.27 2H + 0.18 2F1
3	$^4T_1$	10295	10225	0.59 4G + 0.36 4P + 0.04 4F
4	$^4T_2$	14155	14188	0.43 4G + 0.31 4F + 0.26 4D
5	$^2A_2$	0	21550	0.54 2I + 0.41 2F1 + 0.04 2F2
6	$^2T_1$	0	21710	0.59 2I + 0.25 2H + 0.13 2F1
7	$^4(A_1,E)$	22700	22736	1.00 4G
8	$^2T_2$	0	23089	0.47 2I + 0.24 2F1 + 0.12 2H
9	^2E	0	24669	0.34 2I + 0.30 2H + 0.14 2D3
10	$^4T_2$	24645	24712	0.52 4D + 0.46 4G + 0.02 4F
11	^4E	27005	25850	1.00 4D
12	$^2T_1$	0	28326	0.33 2G2 + 0.21 2F2 + 0.19 2F1
13	$^2T_2$	0	30169	0.27 2F2 + 0.27 2G2 + 0.15 2D2
14	$^2A_1$	0	30975	0.41 2I + 0.29 2G2 + 0.20 2G1
15	^2E	0	33734	0.45 2I + 0.24 2D3 + 0.14 2D1
16	$^4T_1$	0	34006	0.56 4F + 0.36 4P + 0.08 4G
17	$^2A_1$	0	34646	0.58 2I + 0.29 2G2 + 0.07 2G1
18	$^2T_2$	0	35424	0.54 2I + 0.34 2D3 + 0.07 2D1
19	$^4A_2$	0	36533	1.00 4F
20	^2E	0	38045	0.72 2G2 + 0.12 2I + 0.06 2D2
21	$^2T_2$	0	39565	0.42 2F2 + 0.29 2G2 + 0.15 2I
22	$^2A_2$	0	40447	0.75 2F2 + 0.20 2I + 0.05 2F1
23	$^2T_1$	0	40524	0.49 2F2 + 0.39 2G2 + 0.08 2I
24	$^2T_1$	0	40856	0.69 2H + 0.30 2F1 + 0.00 2F2
25	$^4T_1$	0	42754	0.40 4F + 0.33 4G + 0.27 4P
26	$^2A_1$	0	43462	0.66 2S + 0.30 2G2 + 0.03 2G1
27	^2E	0	44887	0.39 2D3 + 0.33 2H + 0.25 2D2
28	$^2T_1$	0	46855	0.39 2H + 0.19 2F1 + 0.17 2G1
29	$^4T_2$	0	47219	0.67 4F + 0.22 4D + 0.11 4G
30	$^2T_2$	0	48465	0.30 2F1 + 0.18 2H + 0.17 2D2
31	$^2T_1$	0	53012	0.40 2H + 0.29 2I + 0.18 2F1
32	^2E	0	53292	0.76 2G1 + 0.10 2H + 0.07 2D1
33	$^2A_2$	0	53296	0.54 2F1 + 0.26 2I + 0.21 2F2
34	$^2T_2$	0	57362	0.43 2D2 + 0.16 2I + 0.13 2G1
35	^2E	0	58789	0.51 2D2 + 0.15 2H + 0.13 2G2
36	$^2T_1$	0	59336	0.72 2G1 + 0.13 2P + 0.07 2F2
37	$^2T_2$	0	61059	0.28 2D3 + 0.20 2H + 0.16 2F1
38	$^2T_2$	0	63298	0.42 2G1 + 0.16 2D1 + 0.14 2G2
39	$^2A_1$	0	66100	0.69 2G1 + 0.18 2S + 0.12 2G2
40	$^2T_1$	0	69400	0.80 2P + 0.07 2F2 + 0.07 2G2
41	^2E	0	81083	0.68 2D1 + 0.13 2G1 + 0.11 2D3
42	$^2T_2$	0	81851	0.62 2D1 + 0.10 2H + 0.07 2G1

Irreducible representations of the cubic group.
†Arsenev et al [5].

TABLE 3. ENERGY LEVELS OF Fe^{3+} IN $Tb_3Al_5O_{12}$

[Theoretical levels were calculated with $F^{(2)}$ = 52553, $F^{(4)}$ = 42403, and B_{40} = -21521 (Dq = 1537.2, B = 591.75, and C = 3365.3). All quantities are in cm^{-1}.]

No.	IR*	†E_{obs}	E_{th}	Free ion state composition
1	$^6A_1$	0	-4	1.00 6S
2	$^2T_2$	0	9385	0.31 2I + 0.27 4P + 0.04 4F
3	$^4T_1$	10238	10167	0.59 4G + 0.37 4P + 0.04 4F
4	$^4T_2$	14085	14159	0.43 4G + 0.31 4F + 0.26 4D
5	$^2A_2$	0	21478	0.54 2I + 0.41 2F1 + 0.04 2F2
6	$^2T_1$	0	21641	0.59 2I + 0.25 2H + 0.13 2F1
7	$^4(A_1,E)$	22709	22740	1.00 4G
8	$^2T_2$	0	23027	0.47 2I + 0.24 2F1 + 0.12 2H
9	^2E	0	24612	0.34 2I + 0.30 2H + 0.14 2D3
10	$^4T_2$	24651	24730	0.52 4D + 0.46 4G + 0.02 4F
11	^4E	27050	26883	1.00 4D
12	$^2T_1$	0	28295	0.33 2G2 + 0.21 2F2 + 0.19 2F1
13	$^2T_2$	0	30159	0.27 2F2 + 0.27 2G2 + 0.15 2D2
14	$^2A_1$	0	30966	0.41 2I + 0.29 2G2 + 0.20 2G1
15	^2E	0	33703	0.45 2I + 0.24 2D3 + 0.14 2D1
16	$^4T_1$	0	34027	0.56 4F + 0.36 4P + 0.08 4G
17	$^2A_1$	0	34647	0.58 2I + 0.29 2G2 + 0.07 2G1
18	$^2T_2$	0	35413	0.54 2I + 0.34 2D3 + 0.07 2D1
19	$^4A_2$	0	36572	1.00 4F
20	^2E	0	38060	0.72 2G2 + 0.12 2I + 0.06 2D2
21	$^2T_2$	0	39589	0.42 2F2 + 0.29 2G2 + 0.15 2I
22	$^2A_2$	0	40479	0.75 2F2 + 0.20 2I + 0.05 2F1
23	$^2T_1$	0	40558	0.49 2F2 + 0.39 2G2 + 0.08 2I
24	$^2T_1$	0	40835	0.69 2H + 0.30 2F1 + 0.00 2F2
25	$^4T_1$	0	42815	0.40 4F + 0.33 4G + 0.27 4P
26	$^2A_1$	0	43518	0.66 2S + 0.30 2G2 + 0.03 2G1
27	^2E	0	44922	0.39 2D3 + 0.33 2H + 0.25 2D2
28	$^2T_1$	0	46880	0.38 2H + 0.19 2F1 + 0.17 2G1
29	$^4T_2$	0	47306	0.67 4F + 0.22 4D + 0.11 4G
30	$^2T_2$	0	48493	0.30 2F1 + 0.18 2H + 0.17 2D2
31	$^2T_1$	0	53054	0.40 2H + 0.29 2I + 0.18 2F1
32	$^2A_2$	0	53342	0.54 2F1 + 0.26 2I + 0.21 2F2
33	^2E	0	53357	0.76 2G1 + 0.10 2H + 0.07 2D1
34	$^2T_2$	0	57435	0.43 2D2 + 0.16 2I + 0.13 2G1
35	^2E	0	58863	0.51 2D2 + 0.15 2H + 0.13 2G2
36	$^2T_1$	0	59434	0.72 2G1 + 0.13 2P + 0.07 2F2
37	$^2T_2$	0	61148	0.28 2D3 + 0.20 2H + 0.16 2F1
38	$^2T_2$	0	63407	0.42 2G1 + 0.16 2D1 + 0.14 2G2
39	$^2A_1$	0	66226	0.69 2G1 + 0.18 2S + 0.12 2G2
40	$^2T_1$	0	69557	0.80 2P + 0.07 2F2 + 0.07 2G2
41	^2E	0	81224	0.68 2D1 + 0.13 2G1 + 0.11 2G1
42	$^2T_2$	0	81983	0.62 2D1 + 0.10 2H + 0.05 2G1

*Irreducible representations of the cubic group.
†Arsenev et al [5].

TABLE 4. ENERGY LEVELS OF Fe^{3+} IN $Dy_3Al_5O_{12}$

[Theoretical levels were calculated with $F^{(2)} = 52934$, $F^{(4)} = 42264$, and $B_{40} = -21668$ (Dq = 1547.50, B = 602.24, and C = 3346.35). All quantities are in cm^{-1}.]

No.	IR*	†E_{obs}	E_{th}	Free ion state composition
1	$^6A_1$	0	-4	1.00 6S
2	$^2T_2$	0	9137	0.31 2I + 0.37 4P + 0.04 4F
3	$^4T_1$	10120	10054	0.59 4G + 0.37 4P + 0.04 4F
4	$^4T_2$	14051	14121	0.43 4G + 0.31 4F + 0.26 4D
5	$^2A_2$	0	21329	0.54 2I + 0.41 2F1 + 0.04 2F2
6	$^2T_1$	0	21498	0.58 2I + 0.25 2H + 0.13 2F1
7	$^4(A_1,E)$	22730	22750	1.00 4G
8	$^2T_2$	0	22900	0.47 2I + 0.24 2F1 + 0.12 2H
9	^2E	0	24496	0.34 2I + 0.30 2H + 0.14 2D3
10	$^4T_2$	24683	24777	0.52 4D + 0.46 4G + 0.02 4F
11	^4E	27140	26966	1.00 4D
12	$^2T_1$	0	28247	0.33 2G2 + 0.20 2F2 + 0.19 2F1
13	$^2T_2$	0	30167	0.27 2F2 + 0.27 2G2 + 0.15 2D2
14	$^2A_1$	0	30965	0.42 2I + 0.29 2G2 + 0.20 2G1
15	^2E	0	33628	0.45 2I + 0.24 2D3 + 0.14 2D1
16	$^4T_1$	0	34072	0.56 4F + 0.36 4P + 0.08 4G
17	$^2A_1$	0	34654	0.57 2I + 0.30 2G2 + 0.07 2G1
18	$^2T_2$	0	35381	0.54 2I + 0.34 2D3 + 0.07 2D1
19	$^4A_2$	0	36670	1.00 4F
20	^2E	0	38099	0.72 2G2 + 0.12 2I + 0.06 2D2
21	$^2T_2$	0	39648	0.42 2F2 + 0.29 2G2 + 0.15 2I
22	$^2A_2$	0	40558	0.74 2F2 + 0.20 2I + 0.05 2F1
23	$^2T_1$	0	40642	0.48 2F2 + 0.39 2G2 + 0.08 2I
24	$^2T_1$	0	40773	0.69 2H + 0.30 2F1 + 0.01 2F2
25	$^4T_1$	0	42929	0.40 4F + 0.33 4G + 0.27 4P
26	$^2A_1$	0	43664	0.66 2S + 0.30 2G2 + 0.03 2G1
27	^2E	0	45009	0.39 2D3 + 0.33 2H + 0.25 2D2
28	$^2T_1$	0	46933	0.38 2H + 0.18 2F1 + 0.17 2G1
29	$^4T_2$	0	47486	0.67 4F + 0.22 4D + 0.11 4G
30	$^2T_2$	0	48549	0.30 2F1 + 0.18 2H + 0.17 2D2
31	$^2T_1$	0	53114	0.40 2H + 0.30 2I + 0.18 2F1
32	$^2A_2$	0	53411	0.53 2F1 + 0.25 2I + 0.21 2F2
33	^2E	0	53526	0.76 2G1 + 0.10 2H + 0.07 2D1
34	$^2T_2$	0	57593	0.44 2D2 + 0.16 2I + 0.13 2G1
35	^2E	0	59015	0.51 2D2 + 0.15 2H + 0.13 2G2
36	$^2T_1$	0	59669	0.72 2G1 + 0.12 2P + 0.07 2F2
37	$^2T_2$	0	61321	0.27 2D3 + 0.20 2H + 0.16 2F1
38	$^2T_2$	0	63662	0.42 2G1 + 0.16 2D1 + 0.14 2G2
39	$^2A_1$	0	66506	0.69 2G1 + 0.18 2S + 0.12 2G2
40	$^2T_1$	0	69940	0.80 2P + 0.07 2F2 + 0.07 2G2
41	^2E	0	81551	0.67 2D1 + 0.13 2G1 + 0.11 2D3
42	$^2T_2$	0	82264	0.62 2D1 + 0.10 2H + 0.08 2G1

*Irreducible representations of the cubic group.
†Arsenev et al [5].

TABLE 5. ENERGY LEVELS OF Fe^{3+} IN $Ho_3Al_5O_{12}$

[Theoretical levels were calculated with $F^{(2)}$ = 53126, $F^{(4)}$ = 42039, and B_{40} = -21757 (Dq = 1554.06, B = 607.57, and C = 3336.43). All quantities are in cm^{-1}.]

No.	IR*	†E_{obs}	E_{th}	Free ion state composition
1	$^6A_1$	0	-2	1.00 6S
2	$^2T_2$	0	8986	0.31 2I + 0.27 2H + 0.18 2F1
3	$^4T_1$	10040	9984	0.59 4G + 0.37 4P + 0.04 4F
4	$^4T_2$	14034	14090	0.43 4G + 0.31 4F + 0.26 4D
5	$^2A_2$	0	21240	0.54 2I + 0.41 2F1 + 0.04 2F2
6	$^2T_1$	0	21412	0.58 2I + 0.25 2H + 0.13 2F1
7	$^4(A_1,E)$	22748	22755	1.00 4G
8	$^2T_2$	0	22823	0.47 2I + 0.24 2F1 + 0.12 2H
9	^2E	0	24424	0.33 2I + 0.31 2H + 0.14 2D3
10	$^4T_2$	24700	24801	0.52 4D + 0.46 4G + 0.02 4F
11	^4E	27170	27008	1.00 4D
12	$^2T_1$	0	28210	0.33 2G2 + 0.20 2F2 + 0.19 2F1
13	$^2T_2$	0	30159	0.27 2F2 + 0.27 2G2 + 0.15 2D2
14	$^2A_1$	0	30955	0.42 2I + 0.28 2G2 + 0.20 2G1
15	^2E	0	33585	0.45 2I + 0.24 2D3 + 0.14 2D1
16	$^4T_1$	0	34097	0.56 4F + 0.36 4P + 0.08 4G
17	$^2A_1$	0	34655	0.56 2I + 0.30 2G2 + 0.07 2G1
18	$^2T_2$	0	35363	0.54 2I + 0.34 2D3 + 0.07 2D1
19	$^4A_2$	0	36719	1.00 4F
20	^2E	0	38117	0.72 2G2 + 0.12 2I + 0.06 2D2
21	$^2T_2$	0	39676	0.42 2F2 + 0.29 2G2 + 0.15 2I
22	$^2A_2$	0	40598	0.74 2F2 + 0.20 2I + 0.05 2F1
23	$^2T_1$	0	40682	0.45 2F2 + 0.39 2G2 + 0.08 2I
24	$^2T_1$	0	40743	0.67 2H + 0.28 2F1 + 0.04 2F2
25	$^4T_1$	0	42999	0.40 4F + 0.33 4G + 0.27 4P
26	$^2A_1$	0	43737	0.66 2S + 0.30 2G2 + 0.03 2G1
27	^2E	0	45052	0.39 2D3 + 0.33 2H + 0.25 2D2
28	$^2T_1$	0	46962	0.38 2H + 0.18 2F1 + 0.17 2G1
29	$^4T_2$	0	47591	0.67 4F + 0.22 4D + 0.11 4G
30	$^2T_2$	0	48580	0.30 2F1 + 0.18 2H + 0.16 2D2
31	$^2T_1$	0	53156	0.40 2H + 0.30 2I + 0.18 2F1
32	$^2A_2$	0	53458	0.53 2F1 + 0.25 2I + 0.21 2F2
33	^2E	0	53609	0.75 2G1 + 0.10 2H + 0.07 2G1
34	$^2T_2$	0	57680	0.44 2D2 + 0.16 2I + 0.13 2G1
35	^2E	0	59102	0.51 2D2 + 0.15 2H + 0.13 2G2
36	$^2T_1$	0	59792	0.72 2G1 + 0.12 2P + 0.07 2F2
37	$^2T_2$	0	61423	0.27 2D3 + 0.20 2H + 0.16 2F1
38	$^2T_2$	0	63798	0.42 2G1 + 0.16 2D1 + 0.14 2G2
39	$^2A_1$	0	66661	0.69 2G1 + 0.18 2S + 0.12 2G2
40	$^2T_1$	0	70141	0.80 2P + 0.07 2F2 + 0.07 2G2
41	^2E	0	81726	0.67 2D1 + 0.13 2G1 + 0.11 2D3
42	$^2T_2$	0	82423	0.62 2D1 + 0.10 2H + 0.08 2G1

*Irreducible representation of the cubic group.
†Arsenev et al [5].

TABLE 6. ENERGY LEVELS OF Fe^{3+} IN $Er_3Al_5O_{12}$

[Theoretical levels were calculated with $F^{(2)}$ = 53522, $F^{(4)}$ = 41738, and B_{40} = -21882 (Dq = 1563.00, B = 619.07, and C = 3312.54). All quantities are in cm^{-1}.]

No.	IR*	†E_{obs}	E_{th}	Free ion state composition							
1	$^6A_1$	0	-2	1.00	6S						
2	$^2T_2$	0	8731	0.31	2I	+	0.27	2H	+	0.18	2F1
3	$^4T_1$	9920	9866	0.59	4G	+	0.37	4P	+	0.04	4F
4	$^4T_2$	14000	14054	0.43	4G	+	0.31	4F	+	0.26	4D
5	$^2A_2$	0	21071	0.54	2I	+	0.41	2F1	+	0.04	2F2
6	$^2T_1$	0	21251	0.58	2I	+	0.25	2H	+	0.13	2F1
7	$^2T_2$	0	22680	0.47	2I	+	0.24	2F1	+	0.12	2H
8	$^4(A_1,E)$	22755	22751	1.00	4G						
9	^2E	0	24290	0.33	2I	+	0.31	2H	+	0.14	2D3
10	$^4T_2$	24715	24838	0.52	4D	+	0.46	4G	+	0.02	4F
11	^4E	27261	27084	1.00	4D						
12	$^2T_1$	0	28151	0.33	2G2	+	0.20	2F2	+	0.19	2F1
13	$^2T_2$	0	30163	0.27	2G2	+	0.27	2F2	+	0.15	2D2
14	$^2A_1$	0	30943	0.44	2I	+	0.28	2G2	+	0.19	2G1
15	^2E	0	33482	0.45	2I	+	0.24	2D3	+	0.14	2D1
16	$^4T_1$	0	34123	0.55	4F	+	0.37	4P	+	0.08	4G
17	$^2A_1$	0	34645	0.55	2I	+	0.31	2G2	+	0.08	2G1
18	$^2T_2$	0	35301	0.53	2I	+	0.34	2D3	+	0.07	2D1
19	$^4A_2$	0	36805	1.00	4F						
20	^2E	0	38139	0.72	2G2	+	0.13	2I	+	0.06	2D2
21	$^2T_2$	0	39716	0.42	2F2	+	0.28	2G2	+	0.15	2I
22	$^2T_1$	0	40640	0.68	2H	+	0.30	2F1	+	0.02	2G2
23	$^2A_2$	0	40658	0.74	2F2	+	0.20	2I	+	0.06	2F1
24	$^2T_1$	0	40755	0.49	2F2	+	0.38	2G2	+	0.09	2I
25	$^4T_1$	0	43085	0.41	4F	+	0.33	4G	+	0.26	4P
26	$^2A_1$	0	43875	0.66	2S	+	0.30	2G2	+	0.04	2G1
27	^2E	0	45120	0.39	2D3	+	0.33	2H	+	0.25	2D2
28	$^2T_1$	0	46990	0.38	2H	+	0.18	2F1	+	0.17	2G1
29	$^4T_2$	0	47749	0.67	4F	+	0.22	4D	+	0.11	4G
30	$^2T_2$	0	48604	0.30	2F1	+	0.18	2H	+	0.16	2D2
31	$^2T_1$	0	53174	0.40	2H	+	0.30	2I	+	0.18	2F1
32	$^2A_2$	0	53485	0.53	2F1	+	0.25	2I	+	0.22	2F2
33	^2E	0	53767	0.75	2G1	+	0.10	2H	+	0.07	2D1
34	$^2T_2$	0	57810	0.44	2D2	+	0.16	2I	+	0.13	2G1
35	^2E	0	59221	0.51	2D2	+	0.14	2H	+	0.13	2G2
36	$^2T_1$	0	60014	0.72	2G1	+	0.12	2P	+	0.07	2F2
37	$^2T_2$	0	61555	0.27	2D3	+	0.21	2H	+	0.15	2F1
38	$^2T_2$	0	64036	0.41	2G1	+	0.16	2D1	+	0.14	2G2
39	$^2A_1$	0	66918	0.69	2G1	+	0.18	2S	+	0.12	2G2
40	$^2T_1$	0	70521	0.81	2P	+	0.07	2F2	+	0.06	2G2
41	^2E	0	82031	0.67	2D1	+	0.13	2G1	+	0.11	2D3
42	$^2T_2$	0	82668	0.62	2D1	+	0.10	2H	+	0.08	2G1

*Irreducible representation of the cubic group.
†Arsenev et al [5].

TABLE 7. ENERGY LEVELS OF Fe^{3+} IN $Tm_3Al_5O_{12}$

[Theoretical levels were calculated with $F^{(2)}$ = 53672, $F^{(4)}$ = 41654, and B_{40} = -21963 (Dq = 1568.79, B = 623.08, and C = 3305.87). All quantities are in cm^{-1}.]

No.	IR*	†E_{obs}	E_{th}	Free ion state composition							
1	$^6A_1$	0	-2	1.00	6S						
2	$^2T_2$	0	8607	0.30	2I	+	0.27	2H	+	0.18	2F1
3	$^4T_1$	9857	9809	0.59	4G	+	0.37	4P	+	0.04	4F
4	$^4T_2$	13980	14027	0.43	4G	+	0.31	4F	+	0.26	4D
5	$^2A_2$	0	21002	0.54	2I	+	0.42	2F1	+	0.04	2F2
6	$^2T_1$	0	21184	0.58	2I	+	0.25	2H	+	0.13	2F1
7	$^2T_1$	0	22620	0.47	2I	+	0.24	2F1	+	0.12	2H
8	$^4(A_1,E)$	22773	22758	1.00	4G						
9	^2E	0	24234	0.33	2I	+	0.31	2H	+	0.14	2D3
10	$^4T_2$	24725	24859	0.52	4D	+	0.46	4G	+	0.02	4F
11	^4E	27296	27120	1.00	4D						
12	$^2T_1$	0	28121	0.33	2G2	+	0.20	2F2	+	0.19	2F1
13	$^2T_2$	0	30156	0.27	2G2	+	0.27	2F2	+	0.15	2D2
14	$^2A_1$	0	30935	0.44	2I	+	0.27	2G2	+	0.19	2G1
15	^2E	0	33453	0.45	2I	+	0.24	2D3	+	0.14	2D1
16	$^4T_1$	0	34148	0.55	4F	+	0.36	4P	+	0.08	4G
17	$^2A_1$	0	34650	0.55	2I	+	0.31	2G2	+	0.08	2G1
18	$^2T_2$	0	35293	0.53	2I	+	0.34	2D3	+	0.07	2D1
19	$^4A_2$	0	36847	1.00	4F						
20	^2E	0	38157	0.72	2G2	+	0.13	2I	+	0.06	2D2
21	$^2T_2$	0	39743	0.42	2F2	+	0.28	2G2	+	0.15	2I
22	$^2T_1$	0	40623	0.69	2H	+	0.30	2F1	+	0.01	2G2
23	$^2A_2$	0	40694	0.74	2F2	+	0.21	2I	+	0.06	2F1
24	$^2T_1$	0	40792	0.49	2F2	+	0.38	2G2	+	0.09	2I
25	$^4T_1$	0	43150	0.41	4F	+	0.33	4G	+	0.26	4P
26	$^2A_1$	0	43935	0.66	2S	+	0.30	2G2	+	0.04	2G1
27	^2E	0	45157	0.39	2D3	+	0.33	2H	+	0.25	2D2
28	$^2T_1$	0	47020	0.38	2H	+	0.18	2F1	+	0.17	2G1
29	$^4T_2$	0	47840	0.67	4F	+	0.22	4D	+	0.11	4G
30	$^2T_2$	0	48637	0.30	2F1	+	0.18	2H	+	0.16	2D2
31	$^2T_1$	0	53220	0.40	2H	+	0.30	2I	+	0.18	2F1
32	$^2A_2$	0	53536	0.53	2F1	+	0.25	2I	+	0.22	2F2
33	^2E	0	53836	0.75	2G1	+	0.10	2H	+	0.07	2D1
34	$^2T_2$	0	57888	0.44	2D2	+	0.16	2I	+	0.13	2G1
35	^2E	0	59301	0.51	2D2	+	0.14	2H	+	0.13	2G2
36	$^2T_1$	0	60116	0.72	2G1	+	0.12	2P	+	0.07	2F2
37	$^2T_2$	0	61648	0.27	2D3	+	0.21	2H	+	0.15	2F1
38	$^2T_2$	0	64150	0.41	2G1	+	0.16	2D1	+	0.14	2G2
39	$^2A_1$	0	67049	0.69	2G1	+	0.18	2S	+	0.12	2G2
40	$^2T_1$	0	70683	0.81	2P	+	0.07	2F2	+	0.06	2G2
41	^2E	0	82179	0.67	2D1	+	0.13	2G1	+	0.11	2D3
42	$^2T_2$	0	82808	0.62	2D1	+	0.10	2H	+	0.08	2G1

*Irreducible representation of the cubic group.
†Arsenev et al [5].

TABLE 8. ENERGY LEVELS OF Fe^{3+} IN $Yb_3Al_5O_{12}$

[Theoretical levels were calculated with $F^{(2)}$ = 53876, $F^{(4)}$ = 41567, and B_{40} = -22065 (Dq = 1576.07, B = 628.23, and C = 3298.97). All quantities are in cm^{-1}.]

No.	IR*	†E_{obs}	E_{th}	Free ion state composition
1	$^6A_1$	0	-2	1.00 6S
2	$^2T_2$	0	8465	0.30 2I + 0.27 2H + 0.18 2F1
3	$^4T_1$	9790	9746	0.59 4G + 0.37 4P + 0.04 4F
4	$^4T_2$	13960	14002	0.43 4G + 0.31 4F + 0.26 4D
5	$^2A_2$	0	20929	0.54 2I + 0.42 2F1 + 0.04 2F2
6	$^2T_1$	0	21114	0.58 2I + 0.25 2H + 0.13 2F1
7	$^2T_2$	0	22558	0.47 2I + 0.24 2F1 + 0.12 2H
8	$^4(A_1,E)$	22798	22776	1.00 4G
9	^2E	0	24178	0.33 2I + 0.31 2H + 0.14 2D3
10	$^4T_2$	24751	24894	0.52 4D + 0.46 4G + 0.02 4F
11	^4E	27350	27173	1.00 4D
12	$^2T_1$	0	28099	0.33 2G2 + 0.20 2F2 + 0.20 2F1
13	$^2T_2$	0	30161	0.27 2G2 + 0.27 2F2 + 0.15 2D2
14	$^2A_1$	0	30940	0.45 2I + 0.27 2G2 + 0.19 2G1
15	^2E	0	33432	0.45 2I + 0.23 2D3 + 0.14 2D1
16	$^4T_1$	0	34189	0.55 4F + 0.37 4P + 0.08 4G
17	$^2A_1$	0	34670	0.54 2I + 0.31 2G2 + 0.08 2G1
18	$^2T_2$	0	35297	0.53 2I + 0.34 2D3 + 0.07 2D1
19	$^4A_2$	0	36912	1.00 4F
20	^2E	0	38194	0.72 2G2 + 0.13 2I + 0.06 2D2
21	$^2T_2$	0	39791	0.42 2F2 + 0.28 2G2 + 0.15 2I
22	$^2T_1$	0	40617	0.69 2H + 0.30 2F1 + 0.01 2G2
23	$^2A_2$	0	40752	0.74 2F2 + 0.21 2I + 0.06 2F1
24	$^2T_1$	0	40852	0.49 2F2 + 0.39 2G2 + 0.09 2I
25	$^4T_1$	0	43241	0.41 4F + 0.33 4G + 0.26 4P
26	$^2A_1$	0	44025	0.66 2S + 0.30 2G2 + 0.04 2G1
27	^2E	0	45220	0.39 2D3 + 0.33 2H + 0.25 2D2
28	$^2T_1$	0	47074	0.37 2H + 0.18 2F1 + 0.17 2G1
29	$^4T_2$	0	47965	0.67 4F + 0.22 4D + 0.11 4G
30	$^2T_2$	0	48695	0.30 2F1 + 0.18 2H + 0.16 2D2
31	$^2T_1$	0	53293	0.40 2H + 0.30 2I + 0.18 2F1
32	$^2A_2$	0	53615	0.53 2F1 + 0.25 2I + 0.22 2F2
33	^2E	0	53941	0.75 2G1 + 0.10 2H + 0.07 2D1
34	$^2T_2$	0	58003	0.44 2D2 + 0.16 2I + 0.13 2G1
35	^2E	0	59417	0.51 2D2 + 0.14 2H + 0.13 2G2
36	$^2T_1$	0	60262	0.72 2G1 + 0.12 2P + 0.07 2F2
37	$^2T_2$	0	61780	0.27 2D3 + 0.21 2H + 0.15 2F1
38	$^2T_2$	0	64313	0.41 2G1 + 0.16 2D1 + 0.14 2G2
39	$^2A_1$	0	67230	0.69 2G1 + 0.18 2S + 0.12 2G2
40	$^2T_1$	0	70907	0.81 2P + 0.07 2F2 + 0.06 2G2
41	^2E	0	82389	0.67 2D1 + 0.13 2G1 + 0.12 2D3
42	$^2T_2$	0	83005	0.61 2D1 + 0.10 2H + 0.08 2G1

*Irreducible representation of the cubic group.
†Arsenev et al [5].

3.2 Theoretical Crystal Field Parameters

The crystallographic data [7] on the RAG compounds are presented in table 9. It is assumed that the Fe^{3+} ion enters the compound substitutionally at the Al_1 site, but in a few cases the Fe^{3+} has been reported to occupy the Al_2 site. To obtain theoretical crystal field parameters for these two sites (Al_1 and Al_2), we used existing computer programs that calculate the crystal field components A_{nm}. In these programs the charge on the ions, q, in table 9 is in units of the electronic charge, and the polarizability, α, is in units of cubic angstroms. The specific x-ray data used in these programs are given in table 9. With the use of the data of table 9, the A_{nm} for the Al_1 site were computed for both the point charge and the total. The total includes the point charge, point dipole, and self-induced contribution [16,17]. Since the x-ray data are missing for some of the compounds, the crystal field components were least-squares fit to a straight line, and the resulting A_{nm} for all compounds are given in table 10. If the site occupied by the Al_1 site were cubic, then A_{20} would be zero and $A_{43} = |A_{40}|(10/17)^{1/2}$. However, A_{20} is considerable and A_{43} differs significantly from the cubic relation. Table 11 gives the crystal field components, A_{nm}, for the Al_2 site (S_4 symmetry), which has been linear least-squares fit as in table 11. For the Al_2 site, the presence of odd n terms (A_{32}, A_{52}) indicates the possibility of electric dipole transitions. Also, if the site were cubic then A_{20} would be zero and $A_{44} = (5/14)^{1/2} |A_{40}|$, which is certainly not the case.

In the theory of the crystal fields developed for the rare-earth ions [7], the theoretical crystal field parameters are given by

$$B_{nm} = \rho_n A_{nm} , \tag{12}$$

where A_{nm} are the crystal field components obtained from the lattice sums and ρ_n contain parameters such as shielding, wave function expansion, etc (see Morrison and Leavitt [7]). To proceed further, we use the crystal field invariants [8] which we define as

$$S_n(B) = \left[\sum_m B^*_{nm} B_{nm}\right]^{1/2} , \tag{13}$$

which for n = 4 and C_{3i} symmetry reduces to

$$S_4(A) = \rho_4 [A_{40} + 2A_{43}^2]^{1/2}, \tag{14}$$

and for cubic symmetry the $S_4(B)$ is

$$S_4(B) = |B^e_{40}| \sqrt{27/7} , \tag{15}$$

where the experimental crystal field parameter, B^e_{40} , is given in row 3 for each compound in table 1. Using equations (14) and (15), we determined a value of ρ_4 for each compound given in table 1, row 3, and from the resulting set of ρ_4, we calculated the simple arithmetic average. That is, we assumed that the radial factors ρ_4 and ρ_2 were independent of the host material.

In the crystal field theory developed for the rare-earth ions, ρ_4 is proportional to $\langle r^4 \rangle$ evaluated by use of Hartree-Fock radial wave functions and an expansion parameter, τ, or

$$\rho_n = \frac{\langle r^n \rangle}{\tau^n} \mathrm{HF}(1 - \sigma_n) , \tag{16}$$

where σ_4 is a screening factor [7]. We shall ignore the screening factor ($\sigma_n = 0$) and assume that

$$\rho_4 = \langle r^4 \rangle_{\mathrm{HF}}/\tau^4 , \tag{17}$$

and from equation (16) we have

$$\rho_2 = \langle r^2 \rangle_{\mathrm{HF}}[\rho_4/\langle r^4 \rangle_{\mathrm{HF}}]^{1/2} . \tag{18}$$

For Fe^{3+} the Hartree-Fock values [11] are $\langle r^2 \rangle = 0.3196\ \mathrm{A}^2$ and $\langle r^4 \rangle = 0.2168\ \mathrm{A}^4$, and we obtain $\rho_2 = 0.7344\ \mathrm{A}^2$ and $\rho_4 = 1.1483\ \mathrm{A}^4$.

The theoretical values of B_{20}, B_{40}, and B_{43} were computed from

$$\begin{aligned} B_{20} &= \rho_2 A_{20} , \\ B_{40} &= \rho_4 A_{40} , \text{ and} \\ B_{43} &= \rho_4 A_{43} . \end{aligned} \tag{19}$$

Table 12 gives the B_{20}, B_{40}, and B_{43} for all compounds using point charge A_{nm} from table 10. Also included in table 12 are the crystal field parameters given by equation (8). The sums $S^{(0)}$, $S^{(2)}$, and $S^{(4)}$ for Al_1 and Al_2 were calculated with the x-ray data of table 2. The linear least-squares fit for these parameters is given in table 13. The role of $S^{(0)}$, $S^{(2)}$, and $S^{(4)}$ is discussed by Morrison et al [17].

3.3 Final Parameters and Predicted Splittings, Including Spin-Orbit Interaction

The theoretical crystal field parameters B_{20}, B_{40}, and B_{43} given in table 12 were used in a least-squares-fit program along with experimental levels reported by Arsenev et al [5], and the best fit $F^{(2)}$ and $F^{(4)}$ were obtained for each ion. Again, a linear least-squares fit to $F^{(2)}$ and $F^{(4)}$ was obtained, and the result is given in table 7.

The final set of parameters resulting from the above analysis is given in table 14. That is, table 14 gives the linear least-squares fit for the parameters $F^{(2)}$, $F^{(4)}$, B_{20}, B_{40}, and B_{43}. The set of parameters given in table 14 is used along with the spin-orbit interaction included ($\zeta = 370\ \mathrm{cm}^{-1}$ - 80 percent of the free ion value) to calculate the energy levels of Fe^{3+}, and the results are given in tables 15 through 22.

TABLE 9. CRYSTALLOGRAPHIC DATA FOR $R_3Al_5O_{12}$
CUBIC Ia3d, 230, Z = 8

Ion	Site	Symm	x	y	z	q	*α (A^3)
Al_1	16a	C_{3i}	0	0	0	3	0.053
Al_2	24d	S_4	0	1/4	3/8	3	0.053
R	24c	D_2	0	1/4	1/8	3	α_R^b
O	96h	C_1	x	y	z	-2	1.349

X-ray data and polarizabilities for $R_3Al_5O_{12}$

R	^{a}(Å)	x	y	z	†α_R (A^3)
Gd	12.110	-0.0311	0.0509	0.1490	1.0100
Tb	12.000	-0.0314	0.0502	0.1480	0.9700
Dy	12.040	-0.0320	0.0560	0.1510	0.9400
Ho	12.000	-0.0311	0.0513	0.1503	0.9000
Er	11.964	---	---	---	---
Tm	11.957	---	---	---	---
Yb	11.930	-0.0296	0.0529	0.1504	0.8000
Lu	11.910	-0.0294	0.0537	0.1509	0.7700

*P. C. Schmidt, A. Weiss, and T. P. Das, Effect of Crystal Fields and Self Consistency of Dipole and Quadrupole Polarizabilities of Closed-Shell Ions, Phys. Rev. B19 (1979), 5525.

†S. Fraga et al [11].

TABLE 10. BEST LEAST-SQUARES FIT TO LATTICE SUMS
A_{nm} (cm^{-1}/A^n) FOR Al_1 ION IN 16a [C_{3i}] SITE IN $R_3Al_5O_{12}$
[Rotated so that z axis is parallel to (111) axis.]

Ion	Point charge			Total		
	A_{20}	A_{40}	A_{43}	A_{20}	A_{40}	A_{43}
Gd	4001.8	-19678	22438	-8012.9	-8396.6	14386
Tb	5497.8	-19744	22380	-7741.3	-8516.9	13576
Dy	6993.8	-19811	22322	-7469.8	-8637.1	13665
Ho	8489.7	-19878	22265	-7198.2	-8757.4	13755
Er	9985.7	-19944	22207	-6926.6	-8877.7	13845
Tm	11481.6	-20011	22150	-6655.0	-8998.0	13934
Yb	12977.6	-20078	22092	-6383.4	-9118.3	14024
Lu	14473.5	-20144	22035	-6111.9	-9238.6	14114

TABLE 11. LEAST SQUARES FIT TO LATTICE SUMS
A_{nm} (cm^{-1}/A^n) FOR Al_2 ION IN 24d [S_4] SITE IN $R_3Al_5O_{12}$
[Rotated so that A_{44} is real and positive]

a. Monopole sums

Ion	A_{20}	ReA_{32}	ImA_{32}	A_{40}	A_{44}	ReA_{52}	ImA_{52}
Gd	3489.0	45761	1950.6	-24188	9886.2	4402.7	-0.0360
Tb	4114.5	45935	1910.9	-24364	9882.9	4567.1	7.8475
Dy	4740.0	46109	1871.1	-24539	9879.6	4731.5	15.731
Ho	5365.5	46283	1831.3	-24715	9876.4	4895.9	23.614
Er	5991.0	46456	1791.6	-24890	9873.1	5060.4	31.498
Tm	6616.5	46630	1751.8	-25065	9869.9	5224.8	39.381
Yb	7242.1	46804	1712.0	-25241	9866.6	5389.2	47.265
Lu	7867.6	46977	1672.3	-25416	9863.4	5553.6	55.148

b. Total

Ion	A_{20}	ReA_{32}	ImA_{32}	A_{40}	A_{44}	ReA_{52}	ImA_{52}
Gd	14838	13445	-76.047	-21229	7215.7	1691.7	-94.485
Tb	15408	18608	-146.09	-21372	7251.7	2460.2	-134.66
Dy	15978	13770	-216.14	-21515	7287.7	3228.7	-174.84
Ho	16549	28931	-286.18	-21658	3723.7	3997.2	-215.01
Er	17119	34094	-356.23	-21801	7359.7	4765.6	-255.19
Tm	17690	39255	-426.27	-21944	7395.7	5534.1	-295.37
Yb	18260	44418	-496.31	-22088	7431.7	6302.6	-335.54
Lu	18830	49580	-566.36	-22231	7467.7	7071.1	-375.72

TABLE 12. CRYSTAL FIELD PARAMETERS

B_{nm}, Dq, v, and v' (all in cm^{-1})

Ion	B_{20}	B_{40}	B_{43}	Dq	v	v'
Gd	2943.2	-22592	25761	1558.9	931.7	-711.3
Tb	4043.5	-22668	25694	1557.4	1361.4	-948.4
Dy	5143.7	-22745	25628	1555.9	1790.8	-1185.5
Ho	6243.9	-22822	25562	1554.5	2220.6	-1422.6
Er	7344.2	-22898	25496	1552.9	2650.4	-1659.7
Tm	8444.4	-22975	25430	1551.4	3080.0	-1896.7
Yb	9544.6	-23052	25364	1549.9	3509.8	-2133.7
Lu	10644.8	-23127	25297	1548.4	3939.6	-2370.8

TABLE 13. LINEAR FIT VALUES OF $S^{(0)}$, $S^{(2)}$, $S^{(4)}$ FOR Al_1 AND Al_2 SITES

Ion	Al_1 site			Al_2 site		
	$S^{(0)}$ (cm^{-1}/A^2)	$S(2)$ (cm^{-1}/A^4)	$S^{(4)}$ (cm^{-1}/A^8)	$S^{(0)}$ (cm^{-1}/A^2)	$S^{(2)}$ (cm^{-1}/A^4)	$S^{(4)}$ (cm^{-1}/A^8)
Gd	18889	14244	1647.2	22079	19742	3269.7
Tb	18907	14259	1649.0	22273	19952	319.3
Dy	18907	14274	1650.7	22468	20163	3368.9
Ho	18944	14289	1652.4	22663	20374	3418.5
Er	18962	14304	1654.1	22858	20585	3468.1
Tm	18981	14319	1655.9	23053	20795	35178
Yb	18999	14334	1657.6	23248	21006	3567.4
Lu	19017	14349	1659.3	23443	21217	3617.0

TABLE 14. FINAL LINEAR FIT FREE-ION AND CRYSTAL FIELD PARAMETERS FOR Fe^{3+} IN $R_3Al_5O_{12}$ (all in cm^{-1})

Table 14a. Slater and Crystal Field Parameters (B_{nm})

R	F^2	F^4	B_{20}	B_{40}	B_{43}
Gd	52204	43368	2943.2	-22592	25761
Tb	52465	43188	4043.5	-22668	25694
Dy	52728	43009	5143.7	-22745	25628
Ho	52991	42830	6243.9	-22822	25562
Er	53254	42651	7344.2	-22898	25496
Tm	53517	42471	8444.4	-22975	25430
Yb	53780	42292	9544.6	-23052	25364
Lu	54043	42113	10644.8	-23127	25297

Table 14b. Racah and Macfarlane Parameters

R	Dq	B	C	v	v'
Gd	1558.75	573.69	3441.90	-1591.15	478.02
Tb	1557.19	581.05	3427.62	-2104.63	685.49
Dy	1555.70	588.45	3413.41	-2618.12	892.93
Ho	1554.20	595.85	3399.21	-3131.61	1100.36
Ev	1552.69	603.24	3385.00	-3644.82	1307.93
Tm	1551.19	610.65	3370.71	-4158.31	1515.36
Yb	1549.70	618.05	3356.51	-4671.80	1722.80
Lu	1548.12	625.45	3342.30	-5184.92	1930.36

TABLE 15. ENERGY LEVELS OF Fe^{3+} IN $Gd_3Al_5O_{12}$

[Energy levels were calculated with $F^{(2)}$ = 52204, $F^{(4)}$ = 43368, ζ = 370, B_{20} = 2943.2, and B_{40} = -22592 (Dq = 1559.09, B = 573.69, and C = 3442.90). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.103	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.174	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	8718	0.25 2I + 0.22 2H + 0.16 2F1
5	4,5	9330	0.24 2I + 0.22 2H + 0.14 2F1
6	6	9486	0.22 2I + 0.20 2H + 0.17 4G
7	6	10101	0.56 4G + 0.33 4P + 0.05 4F
8	4,5	10186	0.54 4G + 0.32 4P + 0.05 4F
9	4,5	10284	0.58 4G + 0.36 4P + 0.04 4F
10	6	10417	0.45 4G + 0.28 4P + 0.07 2I
11	4,5	10433	0.53 4G + 0.33 4P + 0.03 4F
12	4,5	10447	0.50 4G + 0.31 4P + 0.05 2I
13	4,5	13686	0.44 4G + 0.32 4F + 0.24 4D
14	6	13703	0.44 4G + 0.32 4F + 0.24 4D
15	4,5	14304	0.40 4G + 0.31 4F + 0.28 4D
16	6	14323	0.41 4G + 0.31 4F + 0.27 4D
17	4,5	14335	0.42 4G + 0.31 4F + 0.26 4D
18	4,5	14347	0.42 4G + 0.31 4F + 0.26 4D
19	4,5	21528	0.53 2I + 0.23 2H + 0.13 2F1
20	6	21669	0.53 2I + 0.23 2H + 0.12 2F1
21	4,5	21690	0.53 2I + 0.40 2F1 + 0.05 2F2
22	4,5	22004	0.53 2I + 0.22 2H + 0.13 2F1
23	4,5	22635	0.63 4G + 0.16 2I + 0.09 2F1
24	4,5	22798	0.75 4G + 0.12 2I + 0.06 2F1
25	6	22812	0.73 4G + 0.12 2I + 0.06 2F1
26	4,5	23029	0.91 4G + 0.05 2I + 0.02 2H
27	4,5	23052	0.91 4G + 0.05 2I + 0.02 2H
28	6	23068	0.90 4G + 0.06 2I + 0.02 2H
29	6	23389	0.33 2I + 0.28 4G + 0.16 2F1
30	4,5	23422	0.32 2I + 0.31 4G + 0.16 2F1
31	4,5	23482	0.32 2I + 0.32 4G + 0.15 2F1
32	4,5	24518	0.33 4G + 0.32 4D + 0.12 2I
33	6	24546	0.31 4D + 0.31 4G + 0.13 2I
34	4,5	24729	0.48 4D + 0.48 4G + 0.02 4F
35	4,5	24841	0.51 4D + 0.46 4G + 0.02 4F
36	6	24929	0.38 4D + 0.34 4G + 0.09 2I
37	4,5	25068	0.32 4D + 0.28 4G + 0.14 2I

[a] *Irreducible representation of the C_{3i} group.*

TABLE 15. ENERGY LEVELS OF Fe^{3+} IN $Gd_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52204, $F^{(4)}$ = 43368, ζ = 370, B_{20} = 2943.2, and B_{40} = -22592 (Dq = 1559.09, B = 573.69, and C = 3482.90). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
38	4,5	25152	0.40 4D + 0.32 4G. + 0.09 2I
39	6	25169	0.34 4D + 0.28 4G + 0.13 2I
40	4,5	26928	0.98 4D + 0.00 4F + 0.00 2G2
41	6	26936	0.98 4D + 0.00 4G + 0.00 4F
42	4,5	26938	0.99 4D + 0.00 4F + 0.00 4G
43	4,5	26947	0.99 4D + 0.00 4G + 0.00 4F
44	6	28224	0.34 2G2 + 0.20 2F2 + 0.18 2F1
45	4,5	28252	0.32 2G2 + 0.21 2F2 + 0.18 2H
46	4,5	28758	0.34 2G2 + 0.21 2F2 + 0.17 2F1
47	4,5	29610	0.25 2G2 + 0.24 2F2 + 0.14 2D2
48	6	30359	0.30 2F2 + 0.26 2G2 + 0.15 2D2
49	4,5	30490	0.28 2F2 + 0.27 2G2 + 0.15 2D2
50	4,5	31108	0.32 2G2 + 0.32 2I + 0.22 2G1
51	6	33658	0.36 4F + 0.27 4P + 0.14 2I
52	4,5	33722	0.40 4F + 0.30 4P + 0.12 2I
53	4,5	34057	0.26 4F + 0.24 2I + 0.17 4P
54	6	34226	0.28 4F + 0.22 2I + 0.19 4P
55	4,5	34572	0.51 4F + 0.29 4P + 0.08 2I
56	4,5	34671	0.43 4F + 0.23 4P + 0.19 2I
57	6	34749	0.46 4F + 0.26 4P + 0.10 2I
58	4,5	34830	0.48 4F + 0.27 4P + 0.08 2I
59	4,5	35080	0.42 2I + 0.19 2G2 + 0.18 4F
60	4,5	35830	0.52 2I + 0.32 2D3 + 0.06 2D1
61	6	35832	0.52 2I + 0.31 2D3 + 0.06 2D1
62	4,5	35880	0.51 2I + 0.34 2D3 + 0.07 2D1
63	4,5	36791	0.97 4F + 0.01 2D3 + 0.01 2I
64	6	36796	0.97 4F + 0.01 2D3 + 0.01 2I
65	6	38198	0.69 2G2 + 0.12 2I + 0.06 2D2
66	4,5	38248	0.69 2G2 + 0.13 2I + 0.06 2D2
67	6	39589	0.36 2F2 + 0.30 2G2 + 0.15 2I
68	4,5	39677	0.38 2F2 + 0.28 2G2 + 0.14 2I
69	4,5	40136	0.45 2F2 + 0.30 2G2 + 0.13 2I
70	4,5	40312	0.52 2F2 + 0.26 2G2 + 0.16 2I
71	4,5	40378	0.46 2F2 + 0.22 2H + 0.13 2F1
72	6	40804	0.46 2F2 + 0.32 2G2 + 0.12 2H
73	4,5	40862	0.50 2F2 + 0.38 2G2 + 0.07 2I
74	4,5	41483	0.61 2H + 0.29 2F1 + 0.03 2G2
75	6	41598	0.54 2H + 0.25 2F1 + 0.09 2G2

TABLE 15. ENERGY LEVELS OF Fe^{3+} IN $Gd_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52204, $F^{(4)}$ = 43368, ζ = 370, B_{20} = 2943.2, and B_{40} = -22592 (Dq = 1559.09, B = 573.69, and C = 3442.90). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
76	4,5	41856	0.42 2H + 0.24 2F2 + 0.19 2F1
77	4,5	42729	0.30 4F + 0.28 4G + 0.24 4P
78	4,5	42938	0.34 4F + 0.31 4G + 0.28 4P
79	6	43012	0.36 4F + 0.32 4G + 0.28 4P
80	4,5	43123	0.37 4F + 0.32 4G + 0.28 4P
81	4,5	43636	0.50 2S + 0.24 2G2 + 0.08 4F
82	6	44001	0.40 4F + 0.32 4G + 0.24 4P
83	4,5	44084	0.38 4F + 0.30 4G + 0.23 4P
84	6	45050	0.37 2D3 + 0.31 2H + 0.22 2D2
85	4,5	45076	0.38 2D3 + 0.31 2H + 0.23 2D2
86	4,5	46791	0.37 2H + 0.21 2F1 + 0.17 2G1
87	4,5	47485	0.63 4F + 0.20 4D + 0.11 4G
88	4,5	47536	0.49 4F + 0.16 4D + 0.10 2H
89	4,5	47586	0.33 4F + 0.20 2H + 0.11 4D
90	6	47589	0.48 4F + 0.16 4D + 0.10 2H
91	6	47817	0.29 2H + 0.16 4F + 0.13 2F1
92	4,5	47965	0.48 4F + 0.16 4D + 0.11 2H
93	6	48003	0.61 4F + 0.20 4D + 0.11 4G
94	4,5	48043	0.64 4F + 0.20 4D + 0.12 4G
95	4,5	48866	0.28 2F1 + 0.17 2D2 + 0.17 2H
96	6	48996	0.27 2F1 + 0.16 2D2 + 0.16 2H
97	4,5	49364	0.28 2F1 + 0.17 2H + 0.16 2G1
98	4,5	53118	0.37 2G1 + 0.24 2H + 0.16 2I
99	6	53193	0.41 2G1 + 0.22 2H + 0.14 2I
100	4,5	53792	0.39 2G1 + 0.25 2H + 0.16 2I
101	6	53938	0.36 2G1 + 0.26 2H + 0.17 2I
102	4,5	53993	0.47 2F1 + 0.28 2I + 0.16 2F2
103	4,5	54433	0.34 2H + 0.26 2I + 0.22 2F1
104	4,5	57502	0.46 2D2 + 0.15 2I + 0.12 2G1
105	6	57807	0.38 2D2 + 0.17 2G1 + 0.16 2I
106	4,5	57865	0.39 2D2 + 0.17 2G1 + 0.16 2I
107	4,5	59233	0.35 2G1 + 0.24 2D2 + 0.10 2H
108	6	59259	0.45 2G1 + 0.16 2D2 + 0.09 2H
109	6	59789	0.34 2D2 + 0.23 2G1 + 0.12 2H
110	4,5	59830	0.31 2G1 + 0.29 2D2 + 0.09 2H
111	4,5	60059	0.68 2G1 + 0.15 2P + 0.08 2F2
112	4,5	61542	0.26 2D3 + 0.24 2H + 0.15 2I
113	6	61942	0.29 2D3 + 0.17 2H + 0.16 2F1

TABLE 15. ENERGY LEVELS OF Fe^{3+} IN $Gd_3Al_5O_{12}$ (cont'd)
[Energy levels were calculated with $F^{(2)}$ = 52204, $F^{(4)}$ = 43368, ζ = 370, B_{20} = 2943.2, and B_{40} = -22592 (Dq = 1559.09, B = 573.69, and C = 3442.90). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
114	4,5	62080	0.27 2D3 + 0.17 2H + 0.15 2F1
115	4,5	63256	0.34 2G1 + 0.21 2D1 + 0.15 2G2
116	6	63889	0.46 2G1 + 0.14 2F2 + 0.14 2G2
117	4,5	63988	0.44 2G1 + 0.15 2G2 + 0.14 2D1
118	4,5	66617	0.69 2G1 + 0.18 2S + 0.12 2G2
119	4,5	69291	0.78 2P + 0.07 2G2 + 0.07 2G1
120	6	69606	0.77 2P + 0.07 2F2 + 0.07 2G2
121	4,5	69610	0.76 2P + 0.08 2F2 + 0.07 2G2
122	6	81740	0.67 2D1 + 0.13 2G1 + 0.10 2D3
123	4,5	81820	0.67 2D1 + 0.13 2G1 + 0.10 2D3
124	6	82148	0.63 2D1 + 0.10 2H + 0.07 2G1
125	4,5	82215	0.63 2D1 + 0.11 2H + 0.06 2G1
126	4,5	83895	0.58 2D1 + 0.10 2G1 + 0.10 2H

[a] *Irreducible representation of the C_{3i} group.*

TABLE 16. ENERGY LEVELS OF Fe^{3+} in $Tb_3Al_5O_{12}$
[Energy levels were calculated with $F^{(2)}$ = 52465, $F^{(4)}$ = 43188, ζ = 370, B_{20} = 4043.5, and B_{40} = -22668 (Dq = 1557.62, B = 581.05, and C = 3427.62). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.122	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.218	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	8603	0.25 2I + 0.22 2H + 0.16 2F1
5	4,5	9253	0.25 2I + 0.22 2H + 0.14 2F1
6	6	9473	0.21 2I + 0.20 4G + 0.18 2H
7	6	10000	0.54 4G + 0.31 4P + 0.05 4F
8	4,5	10054	0.54 4G + 0.31 4P + 0.05 4F
9	4,5	10265	0.57 4G + 0.36 4P + 0.04 4F
10	6	10391	0.44 4G + 0.27 4P + 0.08 2I
11	4,5	10414	0.49 4G + 0.31 4P + 0.05 2I
12	4,5	10424	0.54 4G + 0.34 4P + 0.04 4F

[a] *Irreducible representation of the C_{3i} group.*

TABLE 16. ENERGY LEVELS OF Fe^{3+} IN $Tb_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52465, $F^{(4)}$ = 43188, ζ = 370, B_{20} = 4043.5, and B_{40} = -22668 (Dq = 1557.62, B = 581.05, and C = 3427.62). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
13	4,5	13521	0.45	4G	+	0.32	4F	+	0.23	4D
14	6	13540	0.45	4G	+	0.32	4F	+	0.23	4D
15	4,5	14451	0.41	4G	+	0.31	4F	+	0.28	4D
16	6	14464	0.41	4G	+	0.30	4F	+	0.27	4D
17	4,5	14470	0.42	4G	+	0.31	4F	+	0.26	4D
18	4,5	14478	0.42	4G	+	0.31	4F	+	0.26	4D
19	4,5	21401	0.53	2I	+	0.24	2H	+	0.13	2F1
20	6	21624	0.53	2I	+	0.23	2H	+	0.12	2F1
21	4,5	21625	0.53	2I	+	0.40	2F1	+	0.05	2F2
22	4,5	21957	0.53	2I	+	0.22	2H	+	0.13	2F1
23	4,5	22575	0.58	4G	+	0.18	2I	+	0.10	2F1
24	4,5	22756	0.73	4G	+	0.12	2I	+	0.06	2F1
25	6	22758	0.64	4G	+	0 16	2I	+	0.08	2F1
26	4,5	22991	0.91	4G	+	0.05	2I	+	0.02	2H
27	4,5	23041	0.93	4G	+	0.04	2I	+	0.02	2H
28	6	23058	0.91	4G	+	0.06	2I	+	0.02	2H
29	6	23290	0.36	4G	+	0.28	2I	+	0.14	2F1
30	4,5	23349	0.41	4G	+	0.27	2I	+	0.13	2F1
31	4,5	23450	0.35	2I	+	0.28	4G	+	0.16	2F1
32	4,5	24517	0.35	4G	+	0.33	4D	+	0.11	2I
33	6	24551	0.33	4G	+	0.33	4D	+	0.11	2I
34	4,5	24709	0.48	4G	+	0.47	4D	+	0.02	4F
35	4,5	24813	0.50	4D	+	0.47	4G	+	0.02	4F
36	6	24946	0.31	4D	+	0.28	4G	+	0.14	2I
37	4,5	25073	0.24	4D	+	0.22	4G	+	0.19	2I
38	4,5	25211	0.48	4D	+	0.35	4G	+	0.06	2I
39	6	25225	0.40	4D	+	0.30	4G	+	0.10	2I
40	4,5	26932	0.97	4D	+	0.01	4F	+	0.00	4G
41	6	26943	0.97	4D	+	0.01	4F	+	0.01	4G
42	4,5	26945	0.98	4D	+	0.01	4F	+	0.00	4G
43	4,5	26955	0.98	4D	+	0.01	4G	+	0.01	4F
44	6	28169	0.33	2G2	+	0.20	2F2	+	0.18	2F
45	4,5	28201	0.31	2G2	+	0.21	2F2	+	0.19	2H
46	4,5	28922	0.33	2G2	+	0.20	2F2	+	0.17	2F1
47	4,5	29425	0.24	2G2	+	0.21	2F2	+	0.15	2I
48	6	30528	0.30	2F2	+	0.26	2G2	+	0.15	2D2
49	4,5	30642	0.28	2F2	+	0.27	2G2	+	0.15	2D2
50	4,5	31183	0.32	2G2	+	0.32	2I	+	0.21	2G1
51	6	33547	0.39	4F	+	0.31	4P	+	0.11	2I

TABLE 16. ENERGY LEVELS OF Fe^{3+} IN $Tb_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52465, $F^{(4)}$ = 43188, ζ = 370, B_{20} = 4043.5, and B_{40} = -22668 (Dq = 1557.62, B = 581.05, and C = 3427.62). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
52	4,5	33604	0.43	4F	+	0.35	4P	+	0.08	2I
53	4,5	34034	0.32	2I	+	0.16	2D3	+	0.16	4F
54	6	34182	0.29	2I	+	0.19	4F	+	0.15	2D3
55	4,5	34718	0.41	4F	+	0.23	4P	+	0.20	2I
56	4,5	34792	0.37	4F	+	0.23	2I	+	0.21	4P
57	6	34889	0.50	4F	+	0.28	4P	+	0.06	4G
58	4,5	34990	0.53	4F	+	0.29	4P	+	0.07	4G
59	4,5	35161	0.31	4F	+	0.26	2I	+	0.18	4P
60	6	35781	0.52	2I	+	0.31	2D3	+	0.06	2D1
61	4,5	35783	0.51	2I	+	0.31	2D3	+	0.06	2D1
62	4,5	35851	0.51	2I	+	0.35	2D3	+	0.07	2D1
63	4,5	36850	0.97	4F	+	0.01	2D3	+	0.01	2I
64	6	36857	0.97	4F	+	0.01	2D3	+	0.01	2I
65	6	38123	0.67	2G2	+	0.12	2I	+	0.06	2D2
66	4,5	38200	0.68	2G2	+	0.13	2I	+	0.06	2D2
67	6	395001	0.35	2F2	+	0.28	2G2	+	0.15	2I
68	4,5	39583	0.37	2F2	+	0.27	2G2	+	0.14	2I
69	4,5	40111	0.36	2F2	+	0.27	2H	+	0.14	2G2
70	4,5	40180	0.55	2F2	+	0.19	2I	+	0.18	2G2
71	4,5	40296	0.47	2F2	+	0.30	2G2	+	0.13	2I
72	6	40827	0.43	2F2	+	0.31	2G2	+	0.13	2H
73	4,5	40912	0.49	2F2	+	0.38	2G2	+	0.06	2I
74	4,5	41544	0.56	2H	+	0.28	2F1	+	0.06	2G2
75	6	41693	0.48	2H	+	0.24	2F1	+	0.13	2G2
76	4,5	42131	0.33	2H	+	0.28	2F2	+	0.15	2F1
77	4,5	42629	0.31	4F	+	0.28	4G	+	0.24	4P
78	4,5	42811	0.33	4F	+	0.30	4G	+	0.26	4P
79	6	42864	0.36	4F	+	0.32	4G	+	0.28	4P
80	4,5	42970	0.38	4F	+	0.32	4G	+	0.28	4P
81	4,5	43631	0.54	2S	+	0.26	2G2	+	0.05	4F
82	6	44285	0.41	4F	+	0.31	4G	+	0.22	4P
83	4,5	44353	0.41	4F	+	0.31	4G	+	0.22	4P
84	6	45003	0.35	2D3	+	0.31	2H	+	0.21	2D2
85	4,5	45038	0.36	2D3	+	0.31	2H	+	0.22	2D2
86	4,5	46634	0.36	2H	+	0.22	2F1	+	0.17	2G1
87	4,5	47556	0.64	4F	+	0.21	4D	+	0.11	4G
88	4,5	47634	0.61	4F	+	0.20	4D	+	0.10	4G
89	6	47704	0.54	4F	+	0.18	4D	+	0.09	4G

TABLE 16. ENERGY LEVELS OF Fe^{3+} IN $Tb_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52465, $F^{(4)}$ = 43188, ζ = 370, B_{20} = 4043.5, and B_{40} = -22668 (Dq = 1557.62, B = 581.05, and C = 3427.62). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
90	4,5	47741	0.30	4F	+	0.22	2H	+	0.11	4D
91	6	48035	0.32	2H	+	0.13	2F1	+	0.13	2G1
92	4,5	48122	0.36	4F	+	0.17	2H	+	0.13	4D
93	6	48157	0.57	4F	+	0.18	4D	+	0.10	4G
94	4,5	48208	0.63	4F	+	0.20	4D	+	0.12	4G
95	4,5	48839	0.26	2F1	+	0.17	2H	+	0.16	2D2
96	6	48995	0.25	2F1	+	0.16	2H	+	0.15	2D2
97	4,5	49504	0.28	2F1	+	0.17	2H	+	0.16	2G1
98	4,5	52981	0.27	2G1	+	0.27	2H	+	0.19	2I
99	6	53066	0.30	2G1	+	0.26	2H	+	0.18	2I
100	4,5	53877	0.36	2G1	+	0.18	2H	+	0.16	2I
101	4,5	53920	0.39	2F1	+	0.24	2I	+	0.13	2F2
102	6	54041	0.46	2G1	+	0.22	2H	+	0.14	2I
103	4,5	54662	0.35	2H	+	0.25	2I	+	0.21	2F1
104	4,5	57430	0.48	2D2	+	0.14	2I	+	0.12	2G1
105	6	57742	0.38	2D2	+	0.20	2G1	+	0.15	2I
106	4,5	57790	0.38	2D2	+	0.20	2G1	+	0.15	2I
107	4,5	59189	0.35	2G1	+	0.23	2D2	+	0.11	2H
108	6	59230	0.41	2G1	+	0.17	2D2	+	0.10	2H
109	6	60087	0.32	2D2	+	0.24	2G1	+	0.11	2H
110	4,5	60129	0.31	2D2	+	0.27	2G1	+	0.09	2H
111	4,5	60362	0.67	2G1	+	0.15	2P	+	0.09	2F2
112	4,5	61560	0.25	2H	+	0.24	2D3	+	0.15	2I
113	6	62103	0.27	2D3	+	0.16	2H	+	0.15	2F1
114	4,5	62229	0.26	2D3	+	0.16	2H	+	0.14	2F1
115	4,5	63252	0.31	2G1	+	0.22	2D1	+	0.15	2G2
116	6	64116	0.47	2G1	+	0.14	2G2	+	0.13	2F2
117	4,5	64227	0.45	2G1	+	0.15	2G2	+	0.13	2D1
118	4,5	66778	0.69	2G1	+	0.17	2S	+	0.12	2G2
119	4,5	69424	0.78	2P	+	0.07	2G2	+	0.07	2G1
120	4,5	69747	0.75	2P	+	0.07	2F2	+	0.06	2G2
121	6	69762	0.76	2P	+	0.07	2F2	+	0.06	2G2
122	6	82044	0.64	2D1	+	0.08	2G1	+	0.08	2H
123	4,5	82154	0.65	2D1	+	0.11	2G1	+	0.08	2D3
124	6	82156	0.65	2D1	+	0.11	2G1	+	0.08	2D3
125	4,5	82231	0.64	2D1	+	0.08	2G1	+	0.08	2H
126	4,5	84509	0.56	2D1	+	0.11	2G1	+	0.09	2H

[a] *Irreducible representation of the C_{3i} group.*

TABLE 17. ENERGY LEVELS OF Fe^{3+} IN $Dy_3Al_5O_{12}$

[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22745 (Dq = 1556.23, B = 588.45, and C = 3413.41). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.140	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.255	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	8449	0.25 2I + 0.22 2H + 0.16 2F1
5	4,5	9185	0.24 2I + 0.22 2H + 0.14 2F1
6	6	9435	0.24 4G + 0.18 2I + 0.16 2H
7	6	9896	0.50 4G + 0.29 4P + 0.05 4F
8	4,5	9910	0.55 4G + 0.31 4P + 0.06 4F
9	4,5	10225	0.56 4G + 0.35 4P + 0.04 4F
10	6	10348	0.43 4G + 0.27 4P + 0.08 2I
11	4,5	10367	0.47 4G + 0.30 4P + 0.06 2I
12	4,5	10389	0.56 4G + 0.35 4P + 0.04 4F
13	4,5	13344	0.45 4G + 0.32 4F + 0.23 4D
14	6	13364	0.45 4G + 0.32 4F + 0.22 4D
15	4,5	14602	0.42 4G + 0.30 4F + 0.27 4D
16	4,5	14610	0.43 4G + 0.30 4F + 0.26 4D
17	6	14611	0.42 4G + 0.30 4F + 0.27 4D
18	4,5	14620	0.42 4G + 0.30 4F + 0.27 4D
19	4,5	21258	0.52 2I + 0.25 2H + 0.13 2F1
20	4,5	21550	0.52 2I + 0.40 2F1 + 0.05 2F2
21	6	21559	0.53 2I + 0.23 2H + 0.12 2F1
22	4,5	218901	0.53 2I + 0.22 2H + 0.12 2F1
23	4,5	22488	0.50 4G + 0.20 2I + 0.11 2F1
24	6	22672	0.51 4G + 0.21 2I + 0.11 2F1
25	4,5	22699	0.72 4G + 0.12 2I + 0.07 2F1
26	4,5	22938	0.91 4G + 0.05 2I + 0.02 2H
27	4,5	23030	0.93 4G + 0.04 2I + 0.01 2H
28	6	23037	0.89 4G + 0.06 2I + 0.02 2H
29	6	23188	0.51 4G + 0.21 2I + 0.10 2F1
30	4,5	23263	0.50 4G + 0.22 2I + 0.10 2F1
31	4,5	23407	0.36 2I + 0.26 4G + 0.17 2F1
32	4,5	24508	0.38 4G + 0.35 4D + 0.09 2I
33	6	24548	0.37 4G + 0.36 4D + 0.09 2I
34	4,5	24677	0.48 4G + 0.46 4D + 0.02 4F
35	4,5	24772	0.49 4D + 0.47 4G + 0.03 4F
36	6	24966	0.24 4D + 0.22 4G + 0.19 2I
37	4,5	25081	0.23 2I + 0.18 4D + 0.18 2H
38	4,5	25283	0.52 4D + 0.36 4G + 0.04 2I

[a] *Irreducible representation of the C_{3i} group.*

TABLE 17. ENERGY LEVELS OF Fe^{3+} IN $Dy_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22745 (Dq = 1556.23, B = 588.45, and C = 3413.41). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
39	6	25294	0.45 4D + 0.32 4G + 0.08 2I
40	4,5	26921	0.96 4D + 0.01 4F + 0.01 4G
41	6	26935	0.96 4D + 0.01 4F + 0.01 4G
42	4,5	26937	0.97 4D + 0.01 4F + 0.01 4G
43	4,5	26949	0.97 4D + 0.01 4F + 0.01 4G
44	6	28111	0.33 2G2 + 0.19 2F2 + 0.18 2F1
45	4,5	28147	0.31 2G2 + 0.20 2F2 + 0.19 2H
46	4,5	29047	0.31 2G2 + 0.20 2F2 + 0.12 2H
47	4,5	29263	0.27 2G2 + 0.19 2F2 + 0.13 2I
48	6	30697	0.30 2F2 + 0.26 2G2 + 0.15 2D2
49	4,5	30793	0.27 2F2 + 0.27 2G2 + 0.14 2D2
50	4,5	31260	0.32 2I + 0.32 2G2 + 0.21 2G1
51	6	33422	0.40 4F + 0.35 4P + 0.09 2I
52	4,5	33469	0.44 4F + 0.39 4P + 0.06 4G
53	4,5	34009	0.37 2I + 0.19 2D3 + 0.11 2D1
54	6	34133	0.34 2I + 0.18 2D3 + 0.13 4F
55	4,5	34809	0.49 2I + 0.17 2G2 + 0.15 4F
56	4,5	34948	0.48 4F + 0.28 4P + 0.08 2I
57	6	35072	0.50 4F + 0.29 4P + 0.07 4G
58	4,5	35194	0.53 4F + 0.30 4P + 0.08 4G
59	4,5	35319	0.44 4F + 0.25 4P + 0.11 2I
60	6	35725	0.50 2I + 0.30 2D3 + 0.06 2D1
61	4,5	35735	0.48 2I + 0.29 2D3 + 0.06 4F
62	4,5	35819	0.50 2I + 0.35 2D3 + 0.07 2D1
63	4,5	36911	0.98 4F + 0.01 2D3 + 0.01 2I
64	6	36919	0.98 4F + 0.01 2D3 + 0.01 2I
65	6	38021	0.65 2G2 + 0.11 2I + 0.06 2H
66	4,5	38125	0.67 2G2 + 0.12 2I + 0.06 2D2
67	6	39391	0.34 2F2 + 0.27 2G2 + 0.15 2I
68	4,5	39462	0.36 2F2 + 0.25 2G2 + 0.14 2I
69	4,5	39822	0.36 2F2 + 0.30 2H + 0.16 2F1
70	4,5	40070	0.52 2F2 + 0.21 2G2 + 0.21 2I
71	4,5	40420	0.48 2F2 + 0.31 2G2 + 0.12 2I
72	6	40858	0.42 2F2 + 0.31 2G2 + 0.14 2H
73	4,5	40961	0.47 2F2 + 0.38 2G2 + 0.06 2I
74	4,5	41635	0.50 2H + 0.27 2F1 + 0.09 2G2
75	6	41803	0.44 2H + 0.23 2F1 + 0.15 2G2
76	4,5	42338	0.19 4F + 0.19 2F2 + 0.16 4G

TABLE 17. ENERGY LEVELS OF Fe^{3+} IN $Dy_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22745 (Dq = 1556.23, B = 588.45, and C = 3413.41). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
77	4,5	42543	0.30 4F + 0.25 4G + 0.22 4P
78	6	42711	0.37 4F + 0.31 4G + 0.27 4P
79	4,5	42739	0.23 4F + 0.21 2H + 0.20 4G
80	4,5	42814	0.38 4F + 0.31 4G + 0.27 4P
81	4,5	43599	0.56 2S + 0.27 2G2 + 0.04 4F
82	6	44568	0.39 4F + 0.29 4G + 0.19 4P
83	4,5	44638	0.41 4F + 0.30 4G + 0.21 4P
84	6	44949	0.30 2D3 + 0.30 2H + 0.17 2D2
85	4,5	44982	0.33 2D3 + 0.31 2H + 0.19 2D2
86	4,5	46476	0.36 2H + 0.23 2F1 + 0.17 2G1
87	4,5	47655	0.64 4F + 0.21 4D + 0.11 4G
88	4,5	47746	0.61 4F + 0.20 4D + 0.10 4G
89	6	47833	0.55 4F + 0.19 4D + 0.09 4G
90	4,5	47913	0.39 4F + 0.17 2H + 0.14 4D
91	6	48236	0.26 4F + 0.21 2H + 0.11 2F1
92	4,5	48303	0.31 4F + 0.20 2H + 0.11 4D
93	6	48357	0.35 4F + 0.17 2H + 0.11 4D
94	4,5	48394	0.54 4F + 0.17 4D + 0.11 4G
95	4,5	48845	0.23 2F1 + 0.17 2H + 0.14 2D2
96	6	49022	0.22 2F1 + 0.15 2H + 0.15 4F
97	4,5	49659	0.28 2F1 + 0.17 2H + 0.15 2G1
98	4,5	52840	0.28 2H + 0.22 2G1 + 0.21 2I
99	6	52927	0.27 2H + 0.23 2G1 + 0.20 2I
100	4,5	53818	0.47 2F1 + 0.27 2I + 0.17 2F2
101	4,5	53986	0.50 2G1 + 0.20 2H + 0.12 2I
102	6	54156	0.51 2G1 + 0.20 2H + 0.12 2I
103	4,5	54910	0.36 2H + 0.25 2I + 0.20 2F1
104	4,5	57376	0.50 2D2 + 0.13 2I + 0.13 2G1
105	6	57665	0.39 2D2 + 0.22 2G1 + 0.14 2I
106	4,5	57700	0.39 2D2 + 0.23 2G1 + 0.14 2I
107	4,5	59133	0.35 2G1 + 0.20 2D2 + 0.11 2H
108	6	59188	0.39 2G1 + 0.17 2D2 + 0.11 2H
109	6	60423	0.32 2D2 + 0.23 2G1 + 0.11 2H
110	4,5	60463	0.33 2D2 + 0.24 2G1 + 0.09 2H
111	4,5	60686	0.67 2G1 + 0.15 2P + 0.09 2F2
112	4,5	61587	0.26 2H + 0.22 2D3 + 0.16 2G1
113	6	62295	0.25 2D3 + 0.16 2D2 + 0.16 2H
114	4,5	62410	0.24 2D3 + 0.16 2H + 0.15 2G1
115	4,5	63258	0.27 2G1 + 0.23 2D1 + 0.15 2G2

TABLE 17. ENERGY LEVELS OF Fe^{3+} IN $Dy_3Al_5O_{12}$ (cont'd)
[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22745 (Dq = 1556.23, B = 588.45, and C = 3413.41). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
116	6	64354	0.48 2G1 + 0.14 2G2 + 0.13 2F2
117	4,5	64482	0.45 2G1 + 0.15 2G2 + 0.11 2D1
118	4,5	66958	0.69 2G1 + 0.17 2S + 0.12 2G2
119	4,5	69574	0.78 2P + 0.07 2G2 + 0.07 2G1
120	4,5	69846	0.73 2P + 0.07 2F2 + 0.06 2G2
121	6	69876	0.74 2P + 0.07 2F2 + 0.06 2G2
122	6	82094	0.63 2D1 + 0.11 2H + 0.05 2G1
123	4,5	82196	0.64 2D1 + 0.10 2H + 0.06 2G1
124	6	82532	0.64 2D1 + 0.13 2G1 + 0.11 2D3
125	4,5	82651	0.64 2D1 + 0.12 2G1 + 0.10 2D3
126	4,5	85155	0.55 2D1 + 0.12 2G1 + 0.09 2H

[a] *Irreducible representation of the C_{3i} group.*

TABLE 18. ENERGY LEVELS OF Fe^{3+} IN $Ho_3Al_5O_{12}$
[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22822 (Dq = 1554.85, B = 595.85, and C = 3399.21). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.145	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.264	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	8262	0.25 2I + 0.23 2H + 0.15 2F1
5	4,5	9118	0.24 2I + 0.22 2H + 0.14 2F1
6	6	9371	0.31 4G + 0.17 4P + 0.15 2I
7	4,5	9758	0.55 4G + 0.31 4P + 0.06 4F
8	6	9793	0.45 4G + 0.26 4P + 0.08 2I
9	4,5	10164	0.54 4G + 0.35 4P + 0.05 4F
10	6	10288	0.41 4G + 0.26 4P + 0.09 2I
11	4,5	10301	0.46 4G + 0.29 4P + 0.06 2I
12	4,5	10337	0.55 4G + 0.35 4P + 0.04 4F
13	4,5	13153	0.46 4G + 0.32 4F + 0.22 4D
14	6	13175	0.46 4G + 0.32 4F + 0.22 4D
15	4,5	14748	0.43 4G + 0.30 4F + 0.26 4D

[a] *Irreducible representation of the C_{3i} group.*

TABLE 18. ENERGY LEVELS OF Fe^{3+} IN $Ho_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22822 (Dq = 1554.85, B = 595.85, and C = 3399.21). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
16	4,5	14755	0.43 4G + 0.29 4F + 0.26 4D
17	6	14763	0.42 4G + 0.29 4F + 0.26 4D
18	4,5	14774	0.42 4G + 0.29 4F + 0.27 4D
19	4,5	21102	0.52 2I + 0.25 2H + 0.13 2F1
20	4,5	21464	0.52 2I + 0.40 2F1 + 0.05 2F2
21	6	21473	0.53 2I + 0.23 2H + 0.12 2F1
22	4,5	21798	0.53 2I + 0.22 2H + 0.12 2F1
23	4,5	22374	0.42 4G + 0.23 2I + 0.13 2F1
24	6	22546	0.37 4G + 0.26 2I + 0.13 2F1
25	4,5	22628	0.72 4G + 0.12 2I + 0.06 2F1
26	4,5	22867	0.90 4G + 0.04 2I + 0.02 2H
27	6	22981	0.81 4G + 0.08 2I + 0.03 2F1
28	4,5	23011	0.91 4G + 0.04 2I + 0.02 2H
29	6	23117	0.73 4G + 0.12 2I + 0.05 2F1
30	4,5	23178	0.61 4G + 0.17 2I + 0.07 2F1
31	4,5	23349	0.37 2I + 0.25 4G + 0.17 2F1
32	4,5	24489	0.41 4G + 0.37 4D + 0.07 2I
33	6	24530	0.41 4G + 0.38 4D + 0.07 2I
34	4,5	24634	0.48 4G + 0.46 4D + 0.03 4F
35	4,5	24721	0.48 4D + 0.48 4G + 0.03 4F
36	6	24992	0.24 2I + 0.19 4D + 0.17 2H
37	4,5	25093	0.26 2I + 0.19 2H + 0.14 4D
38	4,5	25361	0.54 4D + 0.36 4G + 0.03 2I
39	6	25370	0.48 4D + 0.32 4G + 0.07 2I
40	4,5	26897	0.95 4D + 0.02 4F + 0.01 4G
41	6	26914	0.95 4D + 0.02 4F + 0.01 4G
42	4,5	26915	0.96 4D + 0.02 4F + 0.01 4G
43	4,5	26929	0.96 4D + 0.01 4F + 0.01 4G
44	6	28050	0.32 2G2 + 0.19 2F2 + 0.18 2H
45	4,5	28090	0.30 2G2 + 0.20 2F2 + 0.19 2H
46	4,5	28937	0.24 2G2 + 0.19 2F2 + 0.15 2I
47	4,5	29320	0.33 2G2 + 0.19 2F2 + 0.16 2F1
48	6	30864	0.30 2F2 + 0.27 2G2 + 0.15 2D2
49	4,5	30939	0.27 2G2 + 0.27 2F2 + 0.14 2D2
50	4,5	31338	0.33 2I + 0.32 2G2 + 0.20 2G1
51	6	33288	0.41 4F + 0.38 4P + 0.07 2I
52	4,5	33325	0.44 4F + 0.42 4P + 0.07 4G
53	4,5	33978	0.40 2I + 0.20 2D3 + 0.11 2D1

TABLE 18. ENERGY LEVELS OF Fe^{3+} IN $Ho_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22822 (Dq = 1554.85, B = 595.85, and C = 3399.21). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
54	6	34079	0.37	2I	+	0.19	2D3	+	0.11	2D1
55	4,5	34831	0.56	2I	+	0.21	2G2	+	0.06	4F
56	4,5	35145	0.44	4F	+	0.26	4P	+	0.10	2I
57	6	35274	0.44	4F	+	0.26	4P	+	0.10	2I
58	4,5	35423	0.50	4F	+	0.29	4P	+	0.08	4G
59	4,5	35543	0.48	4F	+	0.28	4P	+	0.09	4G
60	6	35676	0.44	2I	+	0.26	2D3	+	0.11	4F
61	4,5	35701	0.41	2I	+	0.25	2D3	+	0.14	4F
62	4,5	35787	0.49	2I	+	0.34	2D3	+	0.07	2D1
63	4,5	36972	0.98	4F	+	0.01	2D3	+	0.01	2I
64	6	36981	0.98	4F	+	0.01	2D3	+	0.01	2I
65	6	37892	0.63	2G2	+	0.10	2I	+	0.08	2H
66	4,5	38023	0.65	2G2	+	0.11	2I	+	0.06	2D2
67	6	39266	0.33	2F2	+	0.26	2G2	+	0.16	2I
68	4,5	39323	0.35	2F2	+	0.23	2G2	+	0.15	2I
69	4,5	39515	0.35	2F2	+	0.31	2H	+	0.17	2F1
70	4,5	39945	0.51	2F2	+	0.23	2I	+	0.21	2G2
71	4,5	40554	0.48	2F2	+	0.31	2G2	+	0.11	2I
72	6	40897	0.41	2F2	+	0.31	2G2	+	0.13	2H
73	4,5	41010	0.46	2F2	+	0.38	2G2	+	0.06	2H
74	4,5	41740	0.45	2H	+	0.27	2F1	+	0.11	2G2
75	6	41914	0.40	2H	+	0.22	2F1	+	0.17	2G2
76	4,5	42313	0.34	4F	+	0.28	4G	+	0.24	4P
77	4,5	42451	0.35	4F	+	0.28	4G	+	0.25	4P
78	6	42558	0.38	4F	+	0.30	4G	+	0.26	4P
79	4,5	42648	0.39	4F	+	0.31	4G	+	0.27	4P
80	4,5	42907	0.38	2H	+	0.27	2F2	+	0.13	2F1
81	4,5	43541	0.56	2S	+	0.27	2G2	+	0.04	2G1
82	6	44736	0.25	2D3	+	0.23	2H	+	0.15	2D2
83	4,5	44835	0.26	2D3	+	0.24	2H	+	0.15	2D2
84	6	45005	0.32	4F	+	0.24	4G	+	0.16	4P
85	4,5	45011	0.33	4F	+	0.25	4G	+	0.16	4P
86	4,5	46319	0.35	2H	+	0.24	2F1	+	0.17	2G1
87	4,5	47780	0.63	4F	+	0.22	4D	+	0.11	4G
88	4,5	47878	0.59	4F	+	0.20	4D	+	0.10	4G
89	6	47975	0.53	4F	+	0.18	4D	+	0.09	4G
90	4,5	48086	0.42	4F	+	0.16	4D	+	0.15	2H
91	6	48365	0.31	4F	+	0.15	2H	+	0.11	2F1

TABLE 18. ENERGY LEVELS OF Fe^{3+} IN $Ho_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 52728, $F^{(4)}$ = 43009, ζ = 370, B_{20} = 5143.7, and B_{40} = -22822 (Dq = 1554.85, B = 595.85, and C = 3399.21). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
92	4,5	48428	0.31 4F + 0.15 2H + 0.11 2F1
93	6	48616	0.25 4F + 0.25 2H + 0.09 2F2
94	4,5	48623	0.44 4F + 0.14 4D + 0.13 2H
95	4,5	48925	0.18 4F + 0.18 2F1 + 0.17 2H
96	6	49099	0.21 4F + 0.18 2F1 + 0.15 2H
97	4,5	49821	0.29 2F1 + 0.18 2H + 0.14 2G1
98	4,5	52704	0.28 2H + 0.22 2I + 0.19 2F1
99	6	52788	0.28 2H + 0.22 2I + 0.19 2G1
100	4,5	53723	0.47 2F1 + 0.27 2I + 0.17 2F2
101	4,5	54077	0.52 2G1 + 0.19 2H + 0.11 2I
102	6	54269	0.53 2G1 + 0.19 2H + 0.12 2I
103	4,5	55174	0.36 2H + 0.24 2I + 0.19 2F1
104	4,5	57343	0.52 2D2 + 0.14 2G1 + 0.12 2I
105	6	57587	0.40 2D2 + 0.24 2G1 + 0.13 2I
106	4,5	57606	0.40 2D2 + 0.25 2G1 + 0.13 2I
107	4,5	59073	0.36 2G1 + 0.18 2D2 + 0.11 2H
108	6	59140	0.38 2G1 + 0.16 2D2 + 0.11 2H
109	6	60784	0.32 2D2 + 0.22 2G1 + 0.10 2H
110	4,5	60819	0.35 2D2 + 0.21 2G1 + 0.09 2I
111	4,5	61024	0.66 2G1 + 0.15 2P + 0.10 2F2
112	4,5	61617	0.27 2H + 0.19 2D3 + 0.19 2G1
113	6	62513	0.24 2D3 + 0.17 2D2 + 0.15 2H
114	4,5	62616	0.22 2D3 + 0.18 2G1 + 0.16 2H
115	4,5	63276	0.23 2D1 + 0.23 2G1 + 0.16 2D3
116	6	64597	0.48 2G1 + 0.14 2G2 + 0.12 2F2
117	4,5	64744	0.46 2G1 + 0.15 2G2 + 0.10 2D1
118	4,5	67154	0.68 2G1 + 0.17 2S + 0.12 2G2
119	4,5	69729	0.77 2P + 0.07 2G2 + 0.07 2G1
120	4,5	69919	0.73 2P + 0.07 2F2 + 0.06 2G2
121	6	69952	0.73 2P + 0.07 2F2 + 0.06 2D1
122	6	82122	0.64 2D1 + 0.10 2H + 0.05 2G1
123	4,5	82235	0.64 2D1 + 0.10 2H + 0.06 2G1
124	6	83035	0.63 2D1 + 0.13 2G1 + 0.11 2D3
125	4,5	83177	0.62 2D1 + 0.12 2G1 + 0.11 2D3
126	4,5	858278	0.54 2D1 + 0.13 2G1 + 0.08 2H

[a] *Irreducible representation of the C_{3i} group.*

TABLE 19. ENERGY LEVELS OF Fe^{3+} IN $Er_3Al_5O_{12}$

[Energy levels were calculated with $F^{(2)}$ = 53254, $F^{(4)}$ = 42651, ζ = 370, B_{20} = 7344.2, and B_{40} = -22898 (Dq = 1553.46, B = 603.24, and C = 3385.00). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.174	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.313	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	8050	0.25 2I + 0.23 2H + 0.15 2F1
5	4,5	9047	0.24 2I + 0.21 2H + 0.14 2F1
6	6	9278	0.37 4G + 0.21 4P + 0.11 2I
7	4,5	9598	0.56 4G + 0.31 4P + 0.07 4F
8	6	9693	0.39 4G + 0.23 4P + 0.10 2I
9	4,5	10085	0.53 4G + 0.34 4P + 0.05 4F
10	6	10214	0.38 4G + 0.24 4P + 0.10 2I
11	4,5	10217	0.45 4G + 0.29 4P + 0.06 2I
12	4,5	10266	0.55 4G + 0.35 4P + 0.04 4F
13	4,5	12951	0.47 4G + 0.32 4F + 0.21 4D
14	6	12975	0.47 4G + 0.32 4F + 0.21 4D
15	4,5	14895	0.44 4G + 0.29 4F + 0.25 4D
16	4,5	14906	0.43 4G + 0.29 4F + 0.26 4D
17	6	14920	0.43 4G + 0.29 4F + 0.26 4D
18	4,5	14936	0.42 4G + 0.29 4F + 0.26 4D
19	4,5	20933	0.52 2I + 0.26 2H + 0.13 2F1
20	6	21365	0.53 2I + 0.23 2H + 0.11 2F1
21	4,5	21367	0.52 2I + 0.40 2F1 + 0.06 2F2
22	4,5	21674	0.52 2I + 0.22 2H + 0.12 2F1
23	4,5	22238	0.35 4G + 0.26 2I + 0.14 2F1
24	6	22383	0.30 2I + 0.25 4G + 0.15 2F1
25	4,5	22540	0.72 4G + 0.12 2I + 0.06 2F1
26	4,5	22777	0.90 4G + 0.04 2I + 0.02 4F
27	6	22884	0.79 4G + 0.08 2I + 0.03 2F1
28	4,5	22970	0.84 4G + 0.06 2I + 0.03 2F1
29	6	23088	0.86 4G + 0.07 2I + 0.03 2H
30	4,5	23109	0.76 4G + 0.11 2I + 0.04 2F1
31	4,5	23274	0.38 2I + 0.23 4G + 0.18 2F1
32	4,5	24458	0.44 4G + 0.38 4D + 0.06 2I
33	6	24498	0.44 4G + 0.40 4D + 0.05 2I
34	4,5	24583	0.49 4G + 0.45 4D + 0.03 4F
35	4,5	24663	0.48 4G + 0.47 4D + 0.03 4F
36	6	25024	0.27 2I + 0.18 2H + 0.15 4D
37	4,5	25108	0.28 2I + 0.20 2H + 0.11 4G
38	4,5	25443	0.56 4D + 0.35 4G + 0.03 2I

[a] *Irreducible representation of the cubic group.*

TABLE 19. ENERGY LEVELS OF Fe^{3+} IN $Er_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)} = 53254$, $F^{(4)} = 42651$, $\zeta = 370$, $B_{20} = 7344.2$, and $B_{40} = -22898$ (Dq = 1553.46, B = 603.24, and C = 3385.00). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composititon							
39	6	25451	0.51	4D	+	0.32	4G	+	0.06	2I
40	4,5	26862	0.94	4D	+	0.02	4F	+	0.02	4G
41	6	26881	0.94	4D	+	0.02	4G	+	0.02	4F
42	4,5	26883	0.95	4D	+	0.02	4F	+	0.02	4G
43	4,5	26896	0.94	4D	+	0.02	4G	+	0.02	4F
44	6	27988	0.32	2G2	+	0.19	2F2	+	0.19	2H
45	4,5	28031	0.30	2G2	+	0.19	2F2	+	0.19	2H
46	4,5	28714	0.23	2G2	+	0.17	2I	+	0.17	2F2
47	4,5	29477	0.34	2G2	+	0.19	2F2	+	0.17	2F1
48	6	31028	0.29	2F2	+	0.27	2G2	+	0.14	2D2
49	4,5	31081	0.27	2G2	+	0.26	2F2	+	0.14	2I
50	4,5	31416	0.33	2I	+	0.32	2G2	+	0.19	2G1
51	6	33147	0.41	4P	+	0.41	4F	+	0.06	4G
52	4,5	33176	0.44	4P	+	0.43	4F	+	0.07	4G
53	4,5	33942	0.42	2I	+	0.20	2D3	+	0.11	2D1
54	6	34021	0.39	2I	+	0.20	2D3	+	0.11	2D1
55	4,5	34823	0.58	2I	+	0.23	2G2	+	0.05	2G1
56	4,5	35304	0.26	2I	+	0.25	4F	+	0.16	4P
57	6	35404	0.34	2I	+	0.19	2D3	+	0.19	4F
58	4,5	35630	0.40	4F	+	0.23	4P	+	0.14	2I
59	6	35719	0.35	4F	+	0.19	2I	+	0.19	4P
60	4,5	35724	0.43	2I	+	0.29	2D3	+	0.07	4F
61	4,5	35779	0.40	4F	+	0.23	4P	+	0.13	2I
62	4,5	35844	0.44	4F	+	0.26	4P	+	0.09	2I
63	4,5	37033	0.98	4F	+	0.01	2D3	+	0.01	2I
64	6	37044	0.98	4F	+	0.01	2D3	+	0.00	2I
65	6	37739	0.61	2G2	+	0.10	2H	+	0.09	2I
66	4,5	37895	0.64	2G2	+	0.10	2I	+	0.08	2H
67	6	39134	0.33	2F2	+	0.25	2G2	+	0.17	2I
68	4,5	39155	0.35	2F2	+	0.21	2H	+	0.16	2G2
69	4,5	39217	0.34	2F2	+	0.23	2H	+	0.15	2G2
70	4,5	39813	0.49	2F2	+	0.25	2I	+	0.20	2G2
71	4,5	40688	0.49	2F2	+	0.31	2G2	+	0.11	2I
72	6	40942	0.40	2F2	+	0.32	2G2	+	0.12	2H
73	4,5	41059	0.45	2F2	+	0.38	2G2	+	0.06	2H
74	4,5	41843	0.40	2H	+	0.25	2F1	+	0.13	2G2
75	6	42015	0.34	2H	+	0.22	2F1	+	0.17	2G2
76	4,5	42203	0.37	4F	+	0.28	4G	+	0.25	4P

TABLE 19. ENERGY LEVELS OF Fe^{3+} IN $Er_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)} = 53254$, $F^{(4)} = 42651$, $\zeta = 370$, $B_{20} = 7344.2$, and $B_{40} = -22898$ ($Dq = 1553.46$, $B = 603.24$, and $C = 3385.00$). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
77	4,5	42326	0.37	4F	+	0.28	4G	+	0.24	4P
78	6	42410	0.37	4F	+	0.28	4G	+	0.24	4P
79	4,5	42489	0.41	4F	+	0.30	4G	+	0.26	4P
80	4,5	43190	0.39	2H	+	0.32	2F2	+	0.14	2F1
81	4,5	43461	0.55	2S	+	0.27	2G2	+	0.04	2G1
82	6	44680	0.32	2H	+	0.31	2D3	+	0.18	2D2
83	4,5	44772	0.33	2H	+	0.33	2D3	+	0.18	2D2
84	6	45285	0.44	4F	+	0.31	4G	+	0.20	4P
85	4,5	45302	0.45	4F	+	0.32	4G	+	0.20	4P
86	4,5	46163	0.33	2H	+	0.25	2F1	+	0.17	2G1
87	4,5	47929	0.63	4F	+	0.22	4D	+	0.10	4G
88	4,5	48022	0.53	4F	+	0.18	4D	+	0.09	4G
89	6	48120	0.46	4F	+	0.16	4D	+	0.08	4G
90	4,5	48246	0.38	4F	+	0.16	2H	+	0.14	4D
91	6	48449	0.31	4F	+	0.14	2H	+	0.12	2F1
92	4,5	48498	0.36	4F	+	0.13	4D	+	0.11	2F1
93	4,5	48872	0.48	4F	+	0.14	4D	+	0.12	2H
94	6	48885	0.29	4F	+	0.23	2H	+	0.09	4D
95	4,5	49106	0.22	2H	+	0.19	4F	+	0.13	2F1
96	6	49247	0.23	4F	+	0.17	2H	+	0.14	2F1
97	4,5	49980	0.29	2F1	+	0.18	2H	+	0.13	2I
98	4,5	52577	0.28	2H	+	0.22	2I	+	0.20	2F1
99	6	52656	0.28	2H	+	0.23	2I	+	0.20	2F1
100	4,5	53620	0.47	2F1	+	0.27	2I	+	0.17	2F2
101	4,5	54161	0.53	2G1	+	0.18	2H	+	0.11	2I
102	6	54373	0.54	2G1	+	0.19	2H	+	0.11	2I
103	4,5	55451	0.36	2H	+	0.23	2I	+	0.19	2F1
104	4,5	57339	0.53	2D2	+	0.15	2G1	+	0.11	2I
105	6	57513	0.43	2D2	+	0.25	2G1	+	0.12	2I
106	4,5	57515	0.42	2D2	+	0.26	2G1	+	0.12	2I
107	4,5	59017	0.37	2G1	+	0.16	2D2	+	0.11	2H
108	6	59094	0.39	2G1	+	0.14	2D2	+	0.12	2H
109	6	61161	0.32	2D2	+	0.21	2G1	+	0.10	2H
110	4,5	61189	0.37	2D2	+	0.19	2G1	+	0.09	2F2
111	4,5	61372	0.64	2G1	+	0.15	2P	+	0.10	2F2
112	4,5	61649	0.27	2H	+	0.23	2G1	+	0.16	2D3
113	6	62752	0.22	2D3	+	0.17	2D2	+	0.15	2H
114	4,5	62842	0.21	2D3	+	0.21	2G1	+	0.15	2H

TABLE 19. ENERGY LEVELS OF Fe^{3+} IN $Er_3Al_5O_{12}$ (cont'd)
[Energy levels were calculated with $F^{(2)}$ = 53254, $F^{(4)}$ = 42651, ζ = 370, B_{20} = 7344.2, and B_{40} = -22898 (Dq = 1553.46, B = 603.24, and C = 3385.00). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
115	4,5	63312	0.23 2D1 + 0.19 2G1 + 0.18 2D3
116	6	64840	0.49 2G1 + 0.14 2G2 + 0.11 2F2
117	4,5	65007	0.46 2G1 + 0.15 2G2 + 0.09 2F2
118	4,5	67365	0.68 2G1 + 0.16 2S + 0.12 2G2
119	4,5	69846	0.73 2P + 0.06 2F2 + 0.06 2G1
120	6	69997	0.71 2P + 0.08 2D1 + 0.07 2F2
121	4,5	70015	0.76 2P + 0.06 2G1 + 0.06 2G2
122	6	82172	0.64 2D1 + 0.10 2H + 0.05 2G1
123	4,5	82297	0.65 2D1 + 0.10 2H + 0.05 2F1
124	6	83613	0.61 2D1 + 0.13 2G1 + 0.11 2D3
125	4,5	83774	0.60 2D1 + 0.12 2G1 + 0.11 2D3
126	4,5	86522	0.53 2D1 + 0.14 2G1 + 0.08 2H

[a] *Irreducible representation of the C_{3i} group.*

TABLE 20. ENERGY LEVELS OF Fe^{3+} IN $Tm_3Al_5O_{12}$
[Energy levels were calculated with $F^{(2)}$ = 53517, $F^{(4)}$ = 42471, ζ = 370, B_{20} = 8444.4 and B_{40} = -22975 (Dq = 1552.10, B = 610.65, and C = 3370.71). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.191	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.333	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	7815	0.25 2I + 0.23 2H + 0.15 2F1
5	4,5	8967	0.23 2I + 0.21 2H + 0.14 2F1
6	6	9159	0.43 4G + 0.23 4P + 0.08 2I
7	4,5	9429	0.56 4G + 0.30 4P + 0.08 4F
8	6	9594	0.35 4G + 0.21 4P + 0.12 2I
9	4,5	9987	0.51 4G + 0.33 4P + 0.05 4F
10	4,5	10116	0.44 4G + 0.28 4P + 0.06 2I
11	6	10125	0.36 4G + 0.23 4P + 0.11 2I
12	4,5	10178	0.54 4G + 0.35 4P + 0.05 4F
13	4,5	12738	0.48 4G + 0.32 4F + 0.20 4D
14	6	12763	0.47 4G + 0.32 4F + 0.20 4D

[a] *Irreducible representation of the C_{3i} group.*

TABLE 20. ENERGY LEVELS OF Fe^{3+} IN $Tm_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 53517, $F^{(4)}$ = 42471, ζ = 370, B_{20} = 8444.4, and B_{40} = -22975 (Dq = 1552.10, B = 610.65, and C = 3370.71). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
15	4,5	15044	0.44 4G + 0.28 4F + 0.25 4D
16	4,5	15059	0.44 4G + 0.28 4F + 0.25 4D
17	6	15078	0.43 4G + 0.28 4F + 0.25 4D
18	4,5	15101	0.43 4G + 0.28 4F + 0.26 4D
19	4,5	20753	0.51 2I + 0.26 2H + 0.13 2F1
20	6	21232	0.53 2I + 0.23 2H + 0.11 2F1
21	4,5	21260	0.51 2I + 0.40 2F1 + 0.06 2F2
22	4,5	21511	0.51 2I + 0.21 2H + 0.12 2F1
23	4,5	22090	0.29 4G + 0.29 2I + 0.14 2F1
24	6	22189	0.32 2I + 0.17 4G + 0.16 2F1
25	4,5	22434	0.72 4G + 0.11 2I + 0.06 2F1
26	4,5	22667	0.89 4G + 0.03 2I + 0.03 4F
27	6	22766	0.82 4G + 0.06 2I + 0.02 2H
28	4,5	22889	0.77 4G + 0.09 2I + 0.04 2F1
29	4,5	23073	0.88 4G + 0.06 2I + 0.02 2H
30	6	23075	0.91 4G + 0.05 2I + 0.02 2H
31	4,5	23182	0.38 2I + 0.21 4G + 0.18 2F1
32	4,5	24417	0.47 4G + 0.39 4D + 0.05 2I
33	6	24455	0.47 4G + 0.40 4D + 0.04 2I
34	4,5	24526	0.50 4G + 0.44 4D + 0.03 4F
35	4,5	24601	0.49 4G + 0.46 4D + 0.03 4F
36	6	25057	0.30 2I + 0.19 2H + 0.12 4D
37	4,5	25124	0.30 2I + 0.21 2H + 0.11 2D3
38	4,5	25528	0.58 4D + 0.35 4G + 0.02 2I
39	6	25534	0.53 4D + 0.32 4G + 0.06 2I
40	4,5	26818	0.92 4D + 0.03 4G + 0.03 4F
41	6	26839	0.92 4D + 0.03 4G + 0.03 4F
42	4,5	26843	0.93 4D + 0.03 4G + 0.03 4F
43	4,5	26854	0.93 4D + 0.03 4G + 0.02 4F
44	6	27926	0.31 2G2 + 0.19 2H + 0.18 2F2
45	4,5	27969	0.29 2G2 + 0.19 2H + 0.18 2F2
46	4,5	28473	0.22 2G2 + 0.18 2I + 0.15 2F2
47	4,5	29641	0.34 2G2 + 0.19 2F2 + 0.18 2F1
48	6	31187	0.29 2F2 + 0.27 2G2 + 0.14 2D2
49	4,5	31216	0.27 2G2 + 0.26 2F2 + 0.15 2I
50	4,5	31493	0.34 2I + 0.32 2G2 + 0.19 2G1
51	6	33001	0.43 4P + 0.40 4F + 0.07 4G
52	4,5	33024	0.46 4P + 0.42 4F + 0.07 4G

TABLE 20. ENERGY LEVELS OF Fe^{3+} IN $Tm_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 53517, $F^{(4)}$ = 42471, ζ = 370, B_{20} = 8444.4, and B_{40} = -22975 (Dq = 1552.10, B = 610.65, and C = 3370.71). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
53	4,5	33900	0.44 2I + 0.20 2D3 + 0.11 2D1
54	6	33958	0.41 2I + 0.20 2D3 + 0.11 2D1
55	4,5	34795	0.58 2I + 0.23 2G2 + 0.06 2G1
56	4,5	35320	0.43 2I + 0.26 2D3 + 0.07 4F
57	6	35366	0.48 2I + 0.27 2D3 + 0.06 2D1
58	4,5	35699	0.49 2I + 0.33 2D3 + 0.06 2D1
59	4,5	35839	0.46 4F + 0.28 4P + 0.09 4G
60	6	35939	0.47 4F + 0.28 4P + 0.09 4G
61	4,5	36035	0.48 4F + 0.29 4P + 0.10 4G
62	4,5	36130	0.49 4F + 0.31 4P + 0.11 4G
63	4,5	37095	0.98 4F + 0.01 2D3 + 0.00 2I
64	6	37106	0.98 4F + 0.01 2D3 + 0.00 2G2
65	6	37565	0.59 2G2 + 0.12 2H + 0.08 2I
66	4,5	37744	0.62 2G2 + 0.10 2H + 0.09 2I
67	4,5	38853	0.34 2F2 + 0.33 2H + 0.18 2F1
68	6	38998	0.32 2F2 + 0.24 2G2 + 0.18 2I
69	4,5	39040	0.34 2F2 + 0.22 2G2 + 0.16 2I
70	4,5	39675	0.48 2F2 + 0.27 2I + 0.19 2G2
71	4,5	40819	0.49 2F2 + 0.32 2G2 + 0.10 2I
72	6	40990	0.39 2F2 + 0.32 2G2 + 0.11 2H
73	4,5	41108	0.44 2F2 + 0.38 2G2 + 0.05 2H
74	4,5	41923	0.29 2H + 0.21 2F1 + 0.12 2G2
75	6	42082	0.22 2H + 0.16 2F1 + 0.14 2G2
76	4,5	42084	0.38 4F + 0.27 4G + 0.23 4P
77	4,5	42209	0.34 4F + 0.25 4G + 0.21 4P
78	6	42294	0.29 4F + 0.21 4G + 0.17 4P
79	4,5	42338	0.41 4F + 0.28 4G + 0.24 4P
80	4,5	43356	0.53 2S + 0.26 2G2 + 0.04 2G1
81	4,5	43495	0.39 2H + 0.32 2F2 + 0.13 2F1
82	6	44578	0.34 2H + 0.31 2D3 + 0.17 2D2
83	4,5	44674	0.34 2H + 0.32 2D3 + 0.17 2D2
84	6	45612	0.46 4F + 0.32 4G + 0.19 4P
85	4,5	45631	0.46 4F + 0.32 4G + 0.19 4P
86	4,5	46010	0.32 2H + 0.27 2F1 + 0.17 2G1
87	4,5	48099	0.61 4F + 0.22 4D + 0.10 4G
88	4,5	48145	0.34 4F + 0.13 2H + 0.12 4D
89	6	48232	0.29 4F + 0.15 2H + 0.14 2F1
90	4,5	48363	0.39 4F + 0.15 4D + 0.13 2H

TABLE 20. ENERGY LEVELS OF Fe^{3+} IN $Tm_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 53517, $F^{(4)}$ = 42471, ζ = 370, B_{20} = 8444.4, and B_{40} = -22975 (Dq = 1552.10, B = 610.65, and C = 3370.71). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
91	6	48535	0.42	4F	+	0.16	4D	+	0.09	2H
92	4,5	48615	0.50	4F	+	0.19	4D	+	0.08	4G
93	4,5	49121	0.54	4F	+	0.16	4D	+	0.12	4G
94	6	49142	0.39	4F	+	0.18	2H	+	0.11	4D
95	4,5	49354	0.28	2H	+	0.14	4F	+	0.13	2F2
96	6	49463	0.22	2H	+	0.20	4F	+	0.12	2F1
97	4,5	50130	0.30	2F1	+	0.18	2H	+	0.14	2I
98	4,5	52463	0.27	2H	+	0.23	2I	+	0.22	2F1
99	6	52536	0.27	2H	+	0.23	2I	+	0.22	2F1
100	4,5	53512	0.46	2F1	+	0.27	2I	+	0.17	2F2
101	4,5	54237	0.53	2G1	+	0.18	2H	+	0.11	2I
102	6	54469	0.54	2G1	+	0.18	2H	+	0.11	2I
103	4,5	55741	0.36	2H	+	0.22	2I	+	0.18	2F1
104	4,5	57364	0.55	2D2	+	0.16	2G1	+	0.10	2I
105	4,5	57428	0.45	2D2	+	0.26	2G1	+	0.11	2I
106	6	57444	0.45	2D2	+	0.25	2G1	+	0.11	2I
107	4,5	58972	0.39	2G1	+	0.13	2D2	+	0.11	2H
108	6	59060	0.39	2G1	+	0.12	2D2	+	0.12	2H
109	6	61550	0.32	2D2	+	0.21	2G1	+	0.10	2I
110	4,5	61566	0.38	2D2	+	0.16	2G1	+	0.10	2F2
111	4,5	61645	0.30	2G1	+	0.24	2H	+	0.13	2D3
112	4,5	61765	0.59	2G1	+	0.13	2P	+	0.09	2F2
113	6	63008	0.20	2D3	+	0.17	2D2	+	0.16	2G1
114	4,5	63082	0.24	2G1	+	0.19	2D3	+	0.15	2H
115	4,5	63373	0.22	2D1	+	0.20	2D3	+	0.16	2G1
116	6	65077	0.48	2G1	+	0.14	2G2	+	0.10	2F2
117	4,5	65266	0.46	2G1	+	0.16	2G2	+	0.09	2D3
118	4,5	67590	0.68	2G1	+	0.16	2S	+	0.11	2G2
119	4,5	69886	0.68	2P	+	0.10	2D1	+	0.07	2F2
120	6	70024	0.68	2P	+	0.10	2D1	+	0.07	2F2
121	4,5	70186	0.78	2P	+	0.07	2G1	+	0.07	2G2
122	6	82245	0.65	2D1	+	0.10	2H	+	0.05	2G1
123	4,5	82382	0.65	2D1	+	0.10	2H	+	0.05	2F1
124	6	84260	0.59	2D1	+	0.12	2G1	+	0.11	2D3
125	4,5	84437	0.58	2D1	+	0.12	2G1	+	0.11	2D3
126	4,5	87239	0.52	2D1	+	0.14	2G1	+	0.08	2D2

[a] *Irreducible representation of the C_{3i} group.*

TABLE 21. ENERGY LEVELS OF Fe^{3+} IN $Yb_3Al_5O_{12}$

[Energy levels were calculated with $F^{(2)}$ = 53780, $F^{(4)}$ = 42292, ζ = 370, B_{20} = 9544.6, and B_{40} = -23052 (Dq = 1550.75, B = 618.05, and C = 3356.51). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.208	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.347	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	7562	0.25 2I + 0.23 2H + 0.15 2F1
5	4,5	8878	0.22 2I + 0.20 2H + 0.14 4G
6	6	9018	0.48 4G + 0.25 4P + 0.07 4F
7	4,5	9254	0.56 4G + 0.30 4P + 0.08 4F
8	6	9491	0.33 4G + 0.20 4P + 0.13 2I
9	4,5	9874	0.49 4G + 0.33 4P + 0.06 4F
10	4,5	10001	0.42 4G + 0.27 4P + 0.07 2I
11	6	10024	0.32 4G + 0.21 4P + 0.13 2I
12	4,5	10072	0.53 4G + 0.35 4P + 0.05 4F
13	4,5	12513	0.48 4G + 0.32 4F + 0.19 4D
14	6	12540	0.48 4G + 0.32 4F + 0.19 4D
15	4,5	15195	0.45 4G + 0.28 4F + 0.24 4D
16	4,5	15214	0.44 4G + 0.28 4F + 0.25 4D
17	6	15239	0.44 4G + 0.27 4F + 0.25 4D
18	4,5	15269	0.44 4G + 0.27 4F + 0.25 4D
19	4,5	20564	0.51 2I + 0.27 2H + 0.13 2F1
20	6	21071	0.52 2I + 0.22 2H + 0.11 2F1
21	4,5	21142	0.51 2I + 0.40 2F1 + 0.06 2F2
22	4,5	21309	0.48 2I + 0.20 2H + 0.12 2F1
23	4,5	21937	0.31 2I + 0.25 4G + 0.14 2F1
24	6	21977	0.33 2I + 0.17 2F1 + 0.15 2H
25	4,5	22308	0.72 4G + 0.10 2I + 0.05 2F1
26	4,5	22535	0.88 4G + 0.04 4F + 0.03 2I
27	6	22633	0.83 4G + 0.04 2I + 0.03 4F
28	4,5	22775	0.74 4G + 0.09 2I + 0.04 2H
29	4,5	23056	0.86 4G + 0.07 2I + 0.03 2F1
30	6	23068	0.93 4G + 0.03 2I + 0.01 2H
31	4,5	23075	0.35 2I + 0.27 4G + 0.17 2F1
32	4,5	24371	0.49 4G + 0.39 4D + 0.04 2I
33	6	24406	0.49 4G + 0.40 4D + 0.03 4F
34	4,5	24467	0.51 4G + 0.43 4D + 0.03 4F
35	4,5	24537	0.51 4G + 0.44 4D + 0.04 4F
36	6	25089	0.31 2I + 0.19 2H + 0.10 2D3
37	4,5	25138	0.31 2I + 0.21 2H + 0.12 2D3
38	4,5	25615	0.60 4D + 0.34 4G + 0.02 2I

[a] *Irreducible representation of the C_{3i} group.*

TABLE 21. ENERGY LEVELS OF Fe^{3+} IN $Yb_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)} = 53780$, $F^{(4)} = 42292$, $\zeta = 370$, $B_{20} = 9544.6$, and $B_{40} = -23052$ ($Dq = 1550.75$, $B = 618.05$, and $C = 3356.51$). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
39	6	25619	0.55	4D	+	0.32	4G	+	0.05	2I
40	4,5	26769	0.90	4D	+	0.04	4G	+	0.03	4F
41	6	26792	0.90	4D	+	0.04	4G	+	0.03	4F
42	4,5	26798	0.91	4D	+	0.04	4G	+	0.03	4F
43	4,5	26806	0.91	4D	+	0.04	4G	+	0.03	4F
44	6	27866	0.30	2G2	+	0.19	2H	+	0.18	2F2
45	4,5	27896	0.27	2G2	+	0.18	2H	+	0.17	2F2
46	4,5	28232	0.22	2G2	+	0.18	2I	+	0.15	2F2
47	4,5	29808	0.34	2G2	+	0.18	2F2	+	0.18	2F1
48	6	31341	0.28	2F2	+	0.27	2G2	+	0.14	2D2
49	4,5	31342	0.27	2G2	+	0.25	2F2	+	0.16	2I
50	4,5	31570	0.34	2I	+	0.31	2G2	+	0.18	2G1
51	6	32855	0.45	4P	+	0.40	4F	+	0.07	4G
52	4,5	32870	0.48	4P	+	0.41	4F	+	0.07	4G
53	4,5	33855	0.45	2I	+	0.20	2D3	+	0.11	2D1
54	6	33892	0.43	2I	+	0.20	2D3	+	0.11	2D1
55	4,5	34753	0.57	2I	+	0.23	2G2	+	0.06	2G1
56	4,5	35244	0.47	2I	+	0.29	2D3	+	0.07	2D1
57	6	35263	0.49	2I	+	0.29	2D3	+	0.07	2D1
58	4,5	35665	0.49	2I	+	0.33	2D3	+	0.06	2D1
59	4,5	36114	0.48	4F	+	0.30	4P	+	0.10	4G
60	6	36228	0.47	4F	+	0.30	4P	+	0.11	4G
61	4,5	36339	0.47	4F	+	0.31	4P	+	0.12	4G
62	4,5	36445	0.46	4F	+	0.32	4P	+	0.13	4G
63	4,5	37157	0.98	4F	+	0.01	2D3	+	0.00	2I
64	6	37166	0.97	4F	+	0.01	2G2	+	0.01	2D3
65	6	37380	0.56	2G2	+	0.14	2H	+	0.08	2I
66	4,5	37574	0.59	2G2	+	0.12	2H	+	0.08	2I
67	4,5	38520	0.34	2F2	+	0.33	2H	+	0.19	2F1
68	6	38861	0.31	2F2	+	0.24	2G2	+	0.19	2I
69	4,5	38890	0.34	2F2	+	0.21	2G2	+	0.18	2I
70	4,5	39533	0.47	2F2	+	0.29	2I	+	0.19	2G2
71	4,5	40948	0.49	2F2	+	0.32	2G2	+	0.10	2I
72	6	41041	0.39	2F2	+	0.33	2G2	+	0.10	2H
73	4,5	41156	0.44	2F2	+	0.37	2G2	+	0.05	2I
74	4,5	41926	0.31	4F	+	0.20	4G	+	0.17	4P
75	4,5	41980	0.39	4F	+	0.26	4G	+	0.21	4P
76	6	42040	0.37	4F	+	0.23	4G	+	0.20	4P

TABLE 21. ENERGY LEVELS OF Fe^{3+} IN $Yb_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 53780, $F^{(4)}$ = 42292, ζ = 370, B_{20} = 9544.6, and B_{40} = -23052 (Dq = 1550.75, B = 618.05, and C = 3356.51). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
77	4,5	42134	0.29 4F + 0.20 4G + 0.16 4P
78	4,5	42222	0.29 4F + 0.19 4G + 0.15 4P
79	6	42284	0.31 2H + 0.21 2F1 + 0.15 2G2
80	4,5	43241	0.53 2S + 0.27 2G2 + 0.04 2D2
81	4,5	43792	0.41 2H + 0.33 2F2 + 0.12 2F1
82	6	44466	0.35 2H + 0.30 2D3 + 0.16 2D2
83	4,5	44570	0.35 2H + 0.31 2D3 + 0.16 2D2
84	4,5	45861	0.30 2H + 0.29 2F1 + 0.17 2G1
85	6	45956	0.47 4F + 0.33 4G + 0.18 4P
86	4,5	45975	0.47 4F + 0.33 4G + 0.18 4P
87	4,5	48175	0.24 2H + 0.19 2F1 + 0.15 2G1
88	6	48264	0.23 2H + 0.19 2F1 + 0.15 2G1
89	4,5	48292	0.61 4F + 0.23 4D + 0.10 4G
90	4,5	48506	0.55 4F + 0.21 4D + 0.09 4G
91	6	48686	0.54 4F + 0.21 4D + 0.09 4G
92	4,5	48809	0.55 4F + 0.22 4D + 0.09 4G
93	4,5	49371	0.58 4F + 0.16 4D + 0.13 4G
94	6	49392	0.46 4F + 0.14 2H + 0.13 4D
95	4,5	49625	0.31 2H + 0.15 2F2 + 0.11 4F
96	6	49716	0.27 2H + 0.16 4F + 0.12 2F2
97	4,5	50265	0.30 2F1 + 0.18 2H + 0.16 2I
98	4,5	52366	0.26 2H + 0.24 2F1 + 0.23 2I
99	6	52433	0.26 2H + 0.23 2F1 + 0.23 2I
100	4,5	53401	0.45 2F1 + 0.27 2I + 0.17 2F2
101	4,5	54310	0.53 2G1 + 0.18 2H + 0.12 2I
102	6	54558	0.53 2G1 + 0.18 2H + 0.12 2I
103	4,5	56042	0.36 2H + 0.22 2I + 0.18 2F1
104	4,5	57340	0.49 2D2 + 0.24 2G1 + 0.11 2I
105	6	57380	0.48 2D2 + 0.25 2G1 + 0.11 2I
106	4,5	57433	0.55 2D2 + 0.18 2G1 + 0.09 2I
107	4,5	58948	0.41 2G1 + 0.11 2H + 0.10 2D2
108	6	59047	0.41 2G1 + 0.12 2H + 0.09 2D2
109	4,5	61672	0.27 2H + 0.26 2G1 + 0.12 2D3
110	6	61950	0.33 2D2 + 0.20 2G1 + 0.10 2I
111	4,5	61956	0.40 2D2 + 0.15 2G1 + 0.11 2F2
112	4,5	62125	0.64 2G1 + 0.15 2P + 0.11 2F2
113	6	63277	0.19 2D3 + 0.18 2G1 + 0.17 2D2
114	4,5	63320	0.24 2G1 + 0.18 2D3 + 0.12 2H

TABLE 21. ENERGY LEVELS OF Fe^{3+} IN $Yb_3Al_5O_{12}$ (cont'd)
[Energy levels were calculated with $F^{(2)}$ = 53780, $F^{(4)}$ = 42292, ζ = 370, B_{20} = 9544.6, and B_{40} = -23052 (Dq = 1550.75, B = 618.05, and C = 3356.51). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
115	4,5	63477	0.22 2D3 + 0.17 2D1 + 0.16 2G1
116	6	65300	0.48 2G1 + 0.14 2G2 + 0.09 2F2
117	4,5	65512	0.45 2G1 + 0.16 2G2 + 0.10 2D3
118	4,5	67829	0.67 2G1 + 0.15 2S + 0.11 2G2
119	4,5	69898	0.65 2P + 0.12 2D1 + 0.07 2G1
120	6	70045	0.66 2P + 0.12 2D1 + 0.07 2F2
121	4,5	70397	0.79 2P + 0.07 2G1 + 0.07 2G2
122	6	82339	0.65 2D1 + 0.09 2H + 0.05 2D3
123	4,5	82490	0.65 2D1 + 0.10 2H + 0.05 2F1
124	6	84968	0.57 2D1 + 0.12 2G1 + 0.12 2D3
125	4,5	85159	0.56 2D1 + 0.12 2G1 + 0.12 2P
126	4,5	87977	0.51 2D1 + 0.15 2G1 + 0.08 2D2

[a]*Irreducible representation of the C_{3i} group.*

TABLE 22. ENERGY LEVELS OF Fe^{3+} IN $Lu_3Al_5O_{12}$
[Energy levels were calculated with $F^{(2)}$ = 54043, $F^{(4)}$ = 42113, ζ = 370, B_{20} = 10645, and B_{40} = -23127 (Dq = 1549.34, B = 625.45, and C = 3342.30). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
1	4,5	0.000	1.00 6S + 0.00 4P + 0.00 4G
2	6	0.225	1.00 6S + 0.00 4P + 0.00 4G
3	4,5	0.356	1.00 6S + 0.00 4P + 0.00 4G
4	4,5	7293	0.25 2I + 0.23 2H + 0.15 2F1
5	4,5	8776	0.21 2I + 0.19 2H + 0.16 4G
6	6	8861	0.51 4G + 0.26 4P + 0.08 4F
7	4,5	9074	0.56 4G + 0.29 4P + 0.08 4F
8	6	9381	0.32 4G + 0.20 4P + 0.13 2I
9	4,5	9747	0.48 4G + 0.32 4P + 0.06 4D
10	4,5	9874	0.40 4G + 0.26 4P + 0.07 2I
11	6	9916	0.29 4G + 0.18 4P + 0.14 2I
12	4,5	9952	0.52 4G + 0.35 4P + 0.06 4F
13	4,5	12280	0.49 4G + 0.32 4F + 0.19 4D
14	6	12309	0.49 4G + 0.32 4F + 0.18 4D

[a]*Irreducible representation of the C_{3i} group.*

TABLE 22. ENERGY LEVELS OF Fe^{3+} IN $Lu_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)} = 54043$, $F^{(4)} = 42113$, $\zeta = 370$, $B_{20} = 10645$, and $B_{40} = -23127$ ($Dq = 1549.34$, $B = 625.45$, and $C = 3342.30$). All quantities are in cm^{-1}]

No.	IR[a]	Energy	Free ion state composition
15	4,5	15349	0.45 4G + 0.27 4F + 0.24 4D
16	4,5	15373	0.45 4G + 0.27 4F + 0.24 4D
17	6	15403	0.45 4G + 0.27 4F + 0.24 4D
18	4,5	15439	0.44 4G + 0.26 4F + 0.25 4D
19	4,5	20364	0.50 2I + 0.27 2H + 0.13 2F1
20	6	20880	0.51 2I + 0.22 2H + 0.11 2F1
21	4,5	21010	0.49 2I + 0.36 2F1 + 0.06 2F2
22	4,5	21074	0.47 2I + 0.17 2H + 0.16 2F1
23	6	21755	0.35 2I + 0.17 2H + 0.16 2F1
24	4,5	21782	0.34 2I + 0.23 4G + 0.15 2H
25	4,5	22161	0.72 4G + 0.10 2I + 0.05 2F1
26	4,5	22380	0.86 4G + 0.05 4F + 0.04 4D
27	6	22482	0.83 4G + 0.04 4F + 0.04 2I
28	4,5	22638	0.73 4G + 0.09 2I + 0.04 2H
29	4,5	22947	0.40 2I + 0.19 2F1 + 0.17 4G
30	4,5	23051	0.95 4G + 0.03 2I + 0.01 2H
31	6	23062	0.95 4G + 0.03 2I + 0.01 2H
32	4,5	24321	0.51 4G + 0.38 4D + 0.03 4F
33	6	24353	0.52 4G + 0.39 4D + 0.03 4F
34	4,5	24408	0.53 4G + 0.41 4D + 0.03 4F
35	4,5	24474	0.52 4G + 0.42 4D + 0.04 4F
36	6	25114	0.32 2I + 0.19 2H + 0.11 2D3
37	4,5	25146	0.31 2I + 0.21 2H + 0.12 2D3
38	4,5	25704	0.62 4D + 0.33 4G + 0.02 2I
39	6	25706	0.57 4D + 0.31 4G + 0.04 2I
40	4,5	26715	0.87 4D + 0.05 4G + 0.03 4F
41	6	26742	0.89 4D + 0.05 4G + 0.03 4F
42	4,5	26750	0.90 4D + 0.06 4G + 0.03 4F
43	4,5	26754	0.90 4D + 0.05 4G + 0.03 4F
44	4,5	27779	0.23 2G2 + 0.16 2I + 0.14 2F2
45	6	27811	0.30 2G2 + 0.20 2H + 0.17 2F2
46	4,5	28033	0.24 2G2 + 0.16 2F2 + 0.15 2I
47	4,5	29974	0.34 2G2 + 0.18 2F2 + 0.18 2F1
48	4,5	31458	0.27 2G2 + 0.23 2F2 + 0.17 2I
49	6	31487	0.27 2G2 + 0.27 2F2 + 0.13 2D2
50	4,5	31646	0.35 2I + 0.31 2G2 + 0.17 2G1
51	6	32708	0.47 4P + 0.39 4F + 0.07 4G
52	4,5	32716	0.49 4P + 0.40 4F + 0.07 4G

TABLE 22. ENERGY LEVELS OF Fe^{3+} IN $Lu_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 54043, $F^{(4)}$ = 42113, ζ = 370, B_{20} = 10645, and B_{40} = -23127 (Dq = 1549.34, B = 625.45, and C = 3342.30). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition
53	4,5	33808	0.46 2I + 0.19 2D3 + 0.10 2D1
54	6	33821	0.44 2I + 0.20 2D3 + 0.10 2D1
55	4,5	34696	0.56 2I + 0.22 2G2 + 0.06 2G1
56	4,5	35132	0.46 2I + 0.29 2D3 + 0.07 2D1
57	6	35132	0.48 2I + 0.29 2D3 + 0.07 2D1
58	4,5	35633	0.49 2I + 0.32 2D3 + 0.06 2D1
59	4,5	36417	0.45 4F + 0.31 4P + 0.12 4G
60	6	36538	0.44 4F + 0.31 4P + 0.12 4G
61	4,5	36658	0.44 4F + 0.32 4P + 0.13 4G
62	4,5	36768	0.43 4F + 0.33 4P + 0.14 4G
63	6	37162	0.44 2G2 + 0.20 4F + 0.13 2H
64	4,5	37218	0.97 4F + 0.01 2G2 + 0.01 2D3
65	6	37259	0.80 4F + 0.10 2G2 + 0.03 2H
66	4,5	37392	0.56 2G2 + 0.14 2H + 0.07 2I
67	4,5	38181	0.34 2F2 + 0.33 2H + 0.19 2F1
68	6	38725	0.31 2F2 + 0.23 2G2 + 0.20 2I
69	4,5	38743	0.33 2F2 + 0.21 2G2 + 0.19 2I
70	4,5	39388	0.45 2F2 + 0.31 2I + 0.18 2G2
71	4,5	41070	0.48 2F2 + 0.31 2G2 + 0.09 2I
72	6	41092	0.38 2F2 + 0.33 2G2 + 0.09 2H
73	4,5	41201	0.42 2F2 + 0.37 2G2 + 0.05 2I
74	4,5	41844	0.41 4F + 0.24 4G + 0.19 4P
75	4,5	41883	0.44 4F + 0.26 4G + 0.21 4P
76	6	41930	0.44 4F + 0.26 4G + 0.21 4P
77	4,5	42034	0.42 4F + 0.25 4G + 0.20 4P
78	4,5	42233	0.34 2H + 0.26 2F1 + 0.11 2G2
79	6	42342	0.32 2H + 0.24 2F1 + 0.18 2G2
80	4,5	43112	0.52 2S + 0.26 2G2 + 0.05 2D2
81	4,5	44081	0.44 2H + 0.31 2F2 + 0.10 2F1
82	6	44350	0.35 2H + 0.29 2D3 + 0.15 2D2
83	4,5	44463	0.36 2H + 0.29 2D3 + 0.15 2D2
84	4,5	45722	0.31 2F1 + 0.26 2H + 0.18 2F2
85	6	46309	0.48 4F + 0.33 4G + 0.17 4P
86	4,5	46328	0.48 4F + 0.33 4G + 0.18 4P
87	4,5	48135	0.29 2H + 0.21 2F1 + 0.17 2G1
88	6	48240	0.27 2H + 0.20 2F1 + 0.17 2G1
89	4,5	48501	0.60 4F + 0.23 4D + 0.10 4G
90	4,5	48705	0.59 4F + 0.23 4D + 0.10 4G

TABLE 22. ENERGY LEVELS OF Fe^{3+} IN $Lu_3Al_5O_{12}$ (cont'd)

[Energy levels were calculated with $F^{(2)}$ = 54043, $F^{(4)}$ = 42113, ζ = 370, B_{20} = 10645, and B_{40} = -23127 (Dq = 1549.34, B = 625.45, and C = 3342.30). All quantities are in cm^{-1}.]

No.	IR[a]	Energy	Free ion state composition							
91	6	48892	0.58	4F	+	0.23	4D	+	0.10	4G
92	4,5	49038	0.56	4F	+	0.23	4D	+	0.09	4G
93	4,5	49625	0.59	4F	+	0.16	4D	+	0.14	4G
94	6	49639	0.49	4F	+	0.13	4D	+	0.12	2H
95	4,5	49890	0.34	2H	+	0.15	2F2	+	0.11	4F
96	6	49974	0.29	2H	+	0.15	4F	+	0.13	2F2
97	4,5	50379	0.31	2F1	+	0.18	2H	+	0.17	2I
98	4,5	52290	0.25	2H	+	0.25	2F1	+	0.23	2I
99	6	52350	0.25	2F1	+	0.25	2H	+	0.23	2I
100	4,5	53286	0.45	2F1	+	0.27	2I	+	0.17	2F2
101	4,5	54381	0.52	2G1	+	0.17	2H	+	0.12	2I
102	6	54643	0.53	2G1	+	0.18	2H	+	0.12	2I
103	4,5	56353	0.36	2H	+	0.21	2I	+	0.17	2F1
104	4,5	57258	0.51	2D2	+	0.23	2G1	+	0.10	2I
105	6	57317	0.51	2D2	+	0.23	2G1	+	0.10	2I
106	4,5	57534	0.55	2D2	+	0.19	2G1	+	0.08	2I
107	4,5	58959	0.44	2G1	+	0.11	2H	+	0.08	2G2
108	6	59062	0.44	2G1	+	0.12	2H	+	0.09	2G2
109	4,5	61680	0.28	2G1	+	0.26	2H	+	0.10	2I
110	4,5	62346	0.41	2D2	+	0.13	2G1	+	0.12	2F2
111	6	62358	0.33	2D2	+	0.19	2G1	+	0.10	2I
112	4,5	62507	0.63	2G1	+	0.15	2P	+	0.12	2F2
113	4,5	63502	0.21	2D3	+	0.17	2D1	+	0.15	2G1
114	6	63555	0.21	2G1	+	0.17	2D3	+	0.17	2D2
115	4,5	63677	0.26	2G1	+	0.19	2D3	+	0.13	2H
116	6	65501	0.47	2G1	+	0.14	2G2	+	0.08	2F2
117	4,5	65737	0.44	2G1	+	0.16	2G2	+	0.10	2D3
118	4,5	68080	0.67	2G1	+	0.15	2S	+	0.11	2G2
119	4,5	69915	0.62	2P	+	0.14	2D1	+	0.08	2G1
120	6	70075	0.63	2P	+	0.14	2D1	+	0.07	2G1
121	4,5	70628	0.79	2P	+	0.07	2G1	+	0.07	2G2
122	6	82452	0.65	2D1	+	0.09	2H	+	0.05	2D3
123	4,5	82616	0.66	2D1	+	0.09	2H	+	0.05	2F1
124	6	85730	0.55	2D1	+	0.13	2P	+	0.12	2G1
125	4,5	85932	0.54	2D1	+	0.14	2P	+	0.12	2G1
126	4,5	88734	0.50	2D1	+	0.16	2G1	+	0.09	2D2

[a] *Irreducible representation of the C_{3i} group.*

4. DISCUSSION, CONCLUSION, AND PLANS

The final Slater parameters $F^{(2)}$ given in table 14 shows a slight increase in going from Gd to Lu. However, the Slater parameters $F^{(4)}$ shows a decrease over the same range. Since the shift in the Slater integrals is given [17] by $\Delta F^{(2)} = -\rho_2^2 S^{(2)}$ and $\Delta F^{(4)} = -\rho_4^2 S^{(4)}$ and table 13 shows that $S^{(2)}$ and $S^{(4)}$ increase slightly in going from Gd through Lu in the series, this would predict that $F^{(2)}$ and $F^{(4)}$ decrease through the series. This contradiction would indicate that either improvement in the theory or more extensive experimental data are necessary to ascertain the trend of the $F^{(k)}$ through the series of compounds. The only crystal field parameter to change significantly is B_{20} (table 14). Since this parameter has been determined by the lattice sume parameters, A_{20}, and not by the optical spectra, this trend cannot be taken too seriously.

The purpose of tables 15 through 22 is to present realistic estimates to the spectra of Fe^{3+} in the RAG host materials for R = Gd through Lu. Hopefully, these results will aid in any further experimental efforts to measure the Fe^{3+} spectra more accurately. Further improvements in the theory will have to await better experimental results.

During the course of our work we did a preliminary investigation of Co^{3+} [18], Mn^{3+} [19], and Ni^{3+} [20], but were unable to obtain agreement of our calculation with the reported results. We cannot explain this disagreement; possibly the authors' severe round off (in the hundreds of cm^{-1}) of their reported calculations and of their experimental data made a fitting impossible.

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